

1 **Assessment of Basin-Scale Hydrologic Impacts of CO₂ Sequestration, Illinois Basin**
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Abstract

Finite-element based sharp-interface models of CO₂ injection were constructed for the Illinois Basin in which porosity and permeability were varied with depth from 0.2 to 0.05 and 125 to 5 mD, respectively within the Mount Simon Formation. We used 726 injection wells located near 42 power plants to deliver 80 million metric tons of CO₂/year. After 100 years of continuous injection, deviatoric fluid pressures varied between 4.4 to 16.4 MPa across central and southern part of the Illinois Basin. Maximum deviatoric pressure reached about 46 % of lithostatic levels to the south. The pressure disturbance (> 0.03 MPa) propagated 9-13 km away from the injection wells resulting in significant well-well pressure interference. The CO₂ plumes radial footprint was only 0.5-2 km after 100 years of injection. Net lateral brine displacement was insignificant due to leakage across the Eau Claire confining unit. If CO₂ remains in a separate phase on geologic time scales, it would migrate northward due to buoyancy at a rate of about 6m/1000 years. Because of historic and paleoseismic events in this region, care should be taken to avoid high pore pressures in the southern Illinois Basin. **(189 words)**

Keywords: Mount Simon, Illinois Basin, CO₂, earthquakes, pressure, brine transport

1. Introduction

The Illinois Basin hosts dozens of coal fired power plants which generates about 300 million metric tons (MT) of CO₂ annually (Fig. 1). As part of the Department of Energy's Geological Sequestration Regional Partnership program, the Midwest Geological Sequestration Consortium (MGSC), a partnership that includes the three state geological surveys in the Illinois basin is investigating the technical constraints on the injection of CO₂ into deep (>1.5 km) reservoirs under supercritical conditions. The Mount Simon Sandstone, a Cambrian siliciclastic unit that is present throughout the basin, is a saline water filled aquifer that is a candidate reservoir for geological sequestration. At these depths, the Mount Simon pore fluids are often in excess of 100,000 mg/l (Hanor, 1987; Hanor and McIntosh, 2006). Simple back of the envelope calculation suggests that there is adequate pore space to accommodate this amount of annual CO₂ production. Assuming that CO₂ is emplaced as a supercritical fluid having a density of 500 kg/m³ into a 500m thick Mount Simon sandstone having an average porosity of 10%, 80 million metric tons of CO₂ could displace all of the brines from an area surrounding a well field and would have an approximate aerial footprint of about 1.8 km x 1.8 km each year. Assuming a simple geometry for the Mount Simon and Illinois basin (500 km by 600 km by 500m), this volume of CO₂ injection would result in the displacement of brines out of the center of the Illinois basin towards its outer margins at a rate of about 0.003 m/year. This calculation doesn't account for more rapid solute migration along permeable pathways (e.g. Liu et al. 2004) and must be considered as a minimum estimate.

It is critical to ensure that fluid pressures near the CO₂ injection wells do not exceed 80% of lithostatic levels in order to minimize the potential of hydrofracturing of the overlying Eau Claire confining unit or inducing earthquakes (e.g. Hsieh and Bredehoeft, 1981; Nicholson and Wesson, 1980, Zoback and Harjes, 1997). This is particularly important for the southern Illinois Basin which hosts active seismogenic zones including the Wabash Valley and New Madrid Seismic Zones (Fig. 2A; Eager et al. 2006, Cramer et al. 1992). Carbon-14 dating of sand dikes and other liquefaction features near fault zones suggests that a series of high magnitude (M5-7) earthquakes occurred during the Holocene

across the southern Illinois Basin (Wheeler and Cramer, 2002; Obermeier et al. 1992; Munson et al., 1992; Fig. 2A). The largest historic earthquake on North America is associated with the Reelfoot Rift system (New Madrid Seismic Zone) which northern margin extends into the southern Illinois Basin. Eager et al. (2006) suggest that the tight clustering of recent micro-earthquakes ($\sim M1.1$) along the Wabash Valley Seismic zone may be due to secondary injection of water associated with water floods within the Illinois Basin. Several seismic events (M4.3-M2.8) are believed to be the result of 11 MPa of induced pore pressure associated with pumping of $164 \text{ m}^3/\text{day}$ of hazardous waste into a Class-1 injection into the a basal Paleozoic reservoir (not the Mount Simon Formation) in Ohio (Fig. 2B; Nicholson and Wesson, 1980; Nicholson et al. 1988 ; Seeber et al. 2004). These authors report that these earthquakes occurred 2 km below Mount Simon formation along a previously unmapped Precambrian fault zone. What is troubling is that the induced pore pressures were far below lithostatic levels and that some of the faults within the southern Illinois Basin (Dudzek et al. 2004) are sub-parallel to the maximum horizontal compressive stress direction (bold blue lines, Fig. 2B) (Zoback and Hickman, 1982; Zoback and Zoback, 1989).

There are reasons to be concerned that pore pressures could approach the lithostatic pressure (fracture pressure) as a result of large scale CO_2 injection within the Mount Simon. First, the average permeability of this Cambrian, Mount Simon reservoir is moderate (less than 1000 mD) and decreases with depth as discussed below. Second, 20th century water withdraws from Illinois Basin Cambro-Ordovician aquifer system (which includes the Mount Simon Formation; Walton, 1962) resulted in large regions (50 km by 50 km) of significant sub-hydrostatic fluid pressures (Olcott, 1992) around Chicago (Fig. 3) due to freshwater withdraws and Minneapolis/St. Paul (Lindholm, 1990; Lloyd and Lyke, 1995). The annual withdraws from municipal water supply wells from the Mount Simon aquifer beneath cities of Minneapolis/St Paul (e.g. 277 million metric tons of H_2O ; Fig. 3C) are of the same order of magnitude as the mass of CO_2 generated across the Illinois Basin by coal-fired power plants. Over the past several decades, water withdraws have modified regional groundwater flow patterns and resulted in decrease of as much as 45 m (0.45 MPa) in the Mount Simon sandstone

124 potentiometric surface in a limited area around the Twin Cities of Minneapolis/St. Paul and by over
125 182 m (1.8 MPa) in the Chicago area (Fig. 3A). Would CO₂ injection from more regionally distributed
126 power plants result in comparable increases in heads and modification in groundwater flow directions?
127 While CO₂ injection would presumably occur over a much more distributed area, the Mount Simon is
128 probably less permeable to the south of Chicago where many coal-fired power plants are located.

129
130 The purpose of this study is to assess some of the hydrologic and seismogenic consequences of CO₂
131 injection into the Mount Simon Formation at the sedimentary basin scale. While a number of studies
132 have quantified the effects of CO₂ injection into subsurface reservoirs around the world (e.g.
133 Chadwick et al., 2003; Hovorka et al., 2001; Lu and Lichtner, 2007), these studies have focused on
134 localized regions (up to about 10 km by 10 km by 100m in the x-, y-, and z-directions, respectively)
135 around injection wells and have neglected the impact of injection on the regional flow field. With
136 only one exception (Birkholzer et al. 2007), we are aware of no quantitative models that have been
137 developed to consider the consequences of large-scale CO₂ injection at the sedimentary basin scale. A
138 secondary objective of this study is to demonstrate the efficacy of numerical sharp-interface
139 representations of CO₂ injection. We propose to address several; specific issues regarding basin-scale
140 CO₂ injection in this study:

- 142 1. Will large-scale CO₂ injection result in the generation of near lithostatic pressures in
143 relatively low permeability regions of the Mount Simon Sandstone reservoir or will pressure
144 anomalies be mitigated by leakage across the overlying Eau Claire confining unit?
- 145 2. What is the likely radius of pressure disturbance away from CO₂ injection wells? Will there
146 be significant well-well interference within- or between- injection well centers?
- 147 3. Does CO₂ injection result in significant displacement of brines towards the margins of the
148 basin to the North where the Mount Simon sandstone is exploited as a water resource ?
- 149 4. Will CO₂ injection result in significant vertical brine displacement across the Eau Claire
150 confining unit?

5. Are there optimal regions of the basin that would likely minimize pore pressure generation and the potential for induced seismic activity?

As noted by the ground breaking study of Birkholzer et al. (2007), some of these questions need to be addressed at the sedimentary basin-scale to ensure that unforeseen well-well interactions do not occur while others can be addressed with more localized analysis. We argue below that there are alternatives to using computationally expensive, multi-phase simulators to address these issues at the sedimentary basin scale. Recently, Nordbotten et al. (2004, 2005) argued that simple, analytical models based on sharp-interface theory are of great value in providing order of magnitude estimates of the hydrologic and environmental consequences of CO₂ injection. By using sharp-interface theory, these authors were able to capture much of the relevant physics of the CO₂ injection problem without relying on numerical methods. In this study, we addressed the questions presented above by developing sharp-interface models of CO₂ injection across the Illinois basin. Our calculations are compared to multi-phase models including TOUGH2 (Birkholzer et al. 2007). Our study does not consider the effects of CO₂ leakage along abandoned petroleum wells (Nordbotten et al.; 2004, 2005). We also compare our model results and those of Birkholzer et al. (2007) to single phase analytical solutions of Hantush and Jacob (1955).

2. Study Area

The Illinois Basin is an intercratonic Paleozoic basin which formed in response to thermal subsidence and Appalachian tectonics (Kolata and Nelson, 1990; Beaumont et al., 1988). It is slightly elongated in a NW-SE direction (Fig. 4). It is about ~620 km long, 375 km wide, and over 4.5 km in depth. Our analysis focuses on the basal Cambrian Mount Simon Sandstone reservoir and overlying Eau Claire confining unit which overlies the Precambrian basement (Lloyd and Lykes, 1995). The slope on the Mount Simon is low (0.006; Fig. 5). Mount Simon thickness varies from 50 to 610 m from North to South (Fig. 6). Medina et al. (2008) subdivided the Mount Simon Sandstone into three subunits based primarily on the gamma ray response from borehole geophysical logs (Fig. 7). A generalization of the

subunits is as follows: the upper unit has a relatively high value of gamma ray possibly due the admixture of more argillaceous material resulting from the transition from a high energy, open marine settings to a quieter more clay-rich depositional environment. The middle unit was defined by its lower gamma ray values that result from a cleaner sandstone and probably constitutes the main flow unit, whereas the lowermost unit was defined by gamma ray values that progressively increases with depth to the base of the formation. This increase is due to the increased non-quartz fractions in the formation as the top of the Precambrian basement complex is approached. In this study, we focused on CO₂ injection into the middle unit of the Mount Simon. The Eau Claire Formation, a unit that is dominantly shale, functions as a confining unit over the Mount Simon (Gray stippled pattern, Fig. 7). The Eau Claire thickness varies between 50-100m. Permeability data on the Eau Claire is not plentiful and there is considerable uncertainty in how it changes with depth and with scale (Birkholzer et al. 2007). The few available permeability measurements of Eau Claire permeability range between 1.4×10^{-18} to $6.7 \times 10^{-20} \text{ m}^2$ (0.002 – 0.00067 mD) as reported by Witherspoon et al. (1962), Walton (1962), and Witherspoon and Neuman (1967). Birkholzer et al. (2007) argued that the presence of fractures could increase the effective basin scale vertical permeability of the Eau Claire by about two orders of magnitude. These two units are overlain by a sequence of Ordovician to Pennsylvanian-age sandstones, shales, and carbonate and coal units (Fig. 4). A thin veneer of Pleistocene to Quaternary-age unconsolidated sediments overlies the basin, along the northern glaciated margin, in stream valleys, and the Mississippian Embayment to the south. The surface topography of the basin is relatively subdued, with less than 300 m of relief. The southern margin of the Illinois Basin was deformed during the late Paleozoic through Mesozoic by tectonic uplift of the Pascola Arch and downwarping of the Mississippian Embayment. Uplift was accommodated, in part, by the generation of the Cottage Grove and Rough Creek-Shawneetown fault systems which trend east-west and extends from the Precambrian basement to the surface (Fig. 4). The Wabash Valley fault system was also rejuvenated at this time.

Four prior basin-scale hydrogeologic models within the Illinois Basin have been developed by Bethke et al. (1991), Gupta and Bair (1997), and Breemer et al. (2002), and Birkholzer et al. (2007). The study of Gupta and Bair (1997) presented drill-stem test (DST) data suggesting hydraulic heads within the Mount Simon were near hydrostatic levels (Fig. 8A). Elevated freshwater heads vary from about 200 to -50 meters above sea level (Fig. 8A). Head gradients across the Mount Simon are rather low (0.0003). Within the water table aquifer across the Illinois Basin (not shown), flow is generally from the north to south but with significant local flow systems associated with surface water drainage networks. The Mount Simon formation across the Illinois basin is characterized by lateral high salinity gradients (Fig. 8B-C; Hanor, 1987; McIntosh and Hanor, 2006). Bethke et al. (1991) argued that brines and hydrocarbons migrated through the Illinois Basin over relatively long geologic time scales (millions of years) and over 600 km distance, driven by tectonic uplift of the Ouachitas and Pascola Arch. It is also likely that Pleistocene glaciations have influenced salinity patterns across the Illinois Basin (McIntosh et al. 2004; Schlegel et al. 2008). The Illinois Basin was over run by the Laurentide ice sheets at least twice during the late Pleistocene (see orange solid and dashed lines, Fig 4). Breemer et al. (2002) developed a series of NE-SW cross-sectional hydrologic models across the Illinois basin following the traverse of the Lake Michigan Lobe of the Laurentide Ice Sheet. The goal of this study was to assess the development basal pore pressures conditions beneath the ice sheet to better understand sliding and basal sediment deformation mechanisms beneath this ice lobe. Their results suggest that the asymmetric salinity pattern from north to south may have been caused by ice sheet derived infiltration (Person et al. 2007). Stable isotope composition and Na-Ca-Cl-Br relations of formation waters within the Illinois basin are indicative of evapo-concentrated seawater, suggesting that these Paleozoic-age fluids are relatively stagnant and have not been flushed by meteoric recharge (Stueber and Walter, 1994). Membrane filtration has also been proposed as a mechanism for high brine concentrations within the Illinois Basin (Bredehoeft et al. 1963) although this has not been confirmed by stable isotope data.

Birkholzer et al. (2007) presented models evaluating the basin-scale consequences of CO₂ injection across the Illinois Basin (Figure 9) using a parallel version of TOUGH2. Like this study, these authors considered CO₂ injection into the Mount Simon and overlying Eau Claire confining unit. CO₂ was injected into 26 wells located in the center of the Illinois Basin in south central Illinois and Indiana (Fig. 9). These authors varied the rate of CO₂ injection between 5-15 million metric tons/year/well ($2.7 - 8.2 \cdot 10^4 \text{ m}^3/\text{day}$ assuming a CO₂ density of 500 kg/m^3). They assigned a permeability to the Eau Claire of 10^{-18} m^2 . The permeability of the member of the Mount Simon that received CO₂ was set to 1000 mD. The water saturated aquifer compressibility was assigned of about $7.0 \cdot 10^{-10} \text{ Pa}^{-1}$ based on a long-term pump test results ($S \sim 0.3$). The total thickness of the Mount Simon that received CO₂ was about 95m. Owing to the high permeability of the Mt Simon (1 darcy) computed pressures propagated across the entire Illinois Basin ($> 200 \text{ km}$) after 30 years of continuous injection (Fig. 9A). Pore pressures never exceeded 3 MPa owing to the relatively permeable conditions represented in their model. The separate phase CO₂ plume was confined to a narrow region around the injection well (about 3 km radial distance).

Cores from the Mount Simon sandstone (Cambrian) and its lateral equivalents in Ohio, Michigan, Kentucky, West Virginia, Pennsylvanian and New York were analyzed as part of the Midwest Regional Carbon Sequestration Partnership (MRCSP) (Medina et al. 2008). Porosity data obtained from 128 core analyses and inferred from 189 geophysical logs suggest that pore volume decreases with depth from 0.27 to 0.02 following an Athy-type (Athy, 1930) relationship due to mechanical compaction and diagenetic changes (Figure 10). Medina et al. (2008) used the data presented in Figure 10 to develop a best fit relationship between porosity-depth. Medina et al. (2008) also presented results from a total of 2,472 permeameter tests performed on core samples from Indiana (1,875 data points), Michigan (458 data points), Ohio (131 data points), and Kentucky (8 data points) indicate a log-linear positive relationship between porosity and permeability (Figure 11). Permeability varies between 10,000 to 0.01 mD within the Mount Simon. The average Mount Simon permeability is about 60 mD.

3. Methods

3.1 Analytic Single-Phase Models

Our analysis of the Mount Simon aquifer and Eau Claire confining unit begins by developing simple analytical models of CO₂ injection into a homogenous, isotropic aquifer overlain by a leaky confining unit following the approach of Hantush and Jacob (1955). The approach is idealized because it assumes a single fluid phase under conditions of steady-state leakage across a confining unit. Our single phase assumption is justified by the observation that the CO₂ phase is restricted to a narrow region around the injection well as demonstrated by Birkholzer et al., (2007). The Eau Claire is assigned a constant thickness and permeability. The governing equation describing radial flow under conditions of single phase fluid injection and leakage across an overlying confining unit is given by (Hantush and Jacob, 1955):

$$\frac{S}{T} \frac{\partial s}{\partial t} = \frac{1}{r} \frac{\partial s}{\partial r} + \frac{\partial^2 s}{\partial r^2} - \frac{K'}{Tb'} s \quad (1)$$

where S is the storativity, r is radial distance from the injection well, t is time, s is change in head above hydrostatic, T is aquifer transmissivity, K' is the hydraulic conductivity of the confining unit, and b' is the thickness of the confining unit. These authors solved equation (1) subject to the following boundary conditions:

$$\begin{aligned} s(r = \infty, t) &= 0 \\ r \frac{\partial s}{\partial r} &= -\frac{Q}{2\pi T} \quad \lim_{r \rightarrow 0} \end{aligned} \quad (2)$$

where Q is the volumetric CO₂ injection rate. We assume hydrostatic initial conditions (i.e. s(r, t=0) = 0 m). Hantush and Jacob (1955) found that the solution to equation (1) is given by:

$$s = \frac{Q}{4\pi T} L(u, v) \quad (3)$$

where

$$u = \frac{r^2 S}{4Tt} \quad v = \frac{r}{\beta} \quad \beta = \sqrt{T \frac{b'}{K'}} \quad (4)$$

Values of the function $L(u, v)$ are provided by Walton (1960). We assigned transmissivity, saturated thickness, and leakance values assuming a water saturated phase. We hypothesize that water will be the dominant phase away from the injection well where there is abundant opportunities for leakage. However, we assigned the storage coefficient based on compressibility of the CO_2 phase.

3.2 Sharp-Interface Model

As outlined by Nordbotten et al. (2005, 2008) and demonstrated by Birkholzer et al., (2007) CO_2 injection will result in a largely water wet system with regions of high CO_2 saturation confined to relatively small regions near the injection well annulus. While the sharp interface approach uses only end-point values of relative permeability and phase saturation, detailed comparisons between sharp-interface and multi-phase codes have shown excellent agreement between computed and observed pore pressures and CO_2 plume geometry when common petrophysical parameters are used (Gasda et al. 2008). The main limitation of the sharp-interface approach is its inability to represent the initial dynamics of vertical segregation of phases within a formation, and the limited representation of interformational vertical heterogeneity through expressions for effective relative permeability that result from vertical averaging. Recently, sharp-interface theory has been used to quantify the potential of CO_2 leakage along abandoned oil and gas wells within sedimentary Basins (Nordbotten et al., 2004, 2005). These authors developed analytical solutions based on sharp-interface equations to quantify reservoir injection pressures and supercritical CO_2 lens thickness within a homogenous, isotropic reservoir as well as determine CO_2 losses associated from an adjacent leaky well bore. Because well

density can be quite high in some reservoirs, these authors argued that numerical solutions are impractical. Following Gasda (2008), we have extended the approach of Nordbotten et al. (2004) by developing numerically based on sharp-interface models of CO₂ injection. The rationale for developing a numerical sharp-interface model is to represent the effects of spatial variations in permeability/porosity associated with burial depth and facies heterogeneity within the Mount Simon sandstone.

The governing equations describing CO₂ injection into a leaky, confined aquifer within a sedimentary basin using sharp-interface theory we used here are similar to the methodology outlined by Ledoux et al. (1990). This approach has also been applied to two-phase petroleum systems (Lehner et al., 1987; Rhea et al., 1994). We invoke some restrictive simplifying assumptions in applying sharp-interface theory to the CO₂–brine transport problem. First we assume that the top of the reservoir or carrier bed is flat with an elevation of zero. The CO₂ heads are initially set to zero (i.e. no regional head gradients are imposed). Elevated CO₂ heads are due solely to the effects of supercritical injection (Fig. 12). We will address the effects of buoyancy and hydrodynamic driven flow within the Mount Simon Sandstone on long-range, separate-phase CO₂ migration later using an approach first presented by Hubbert (1953) described below. Gasda's (2008) sharp-interface model has overcome these simplifying assumptions using sharp-interface theory.

In our sharp-interface approach, two, transmissivity-based flow equations describing changes in freshwater head (h_f) as well as the position of the CO₂–brine (z_{ic}) interface are solved (Fig. 12):

CO₂ Transport:

$$(z_t - z_{ic})S_c \frac{\partial h_c}{\partial t} - \phi(1 - S_r) \frac{\partial z_{ic}}{\partial t} = \frac{\partial}{\partial x} \left[T_c \frac{\rho_f}{\rho_c} \frac{\partial h_c}{\partial x} \right] + \frac{\partial}{\partial y} \left[T_c \frac{\rho_f}{\rho_c} \frac{\partial h_c}{\partial y} \right] + q_c \quad (5)$$

Brine Transport:

$$\phi(1 - S_r) \left[\frac{\partial z_{ic}}{\partial t} \right] = \frac{\partial}{\partial x} \left[T_s \frac{\rho_c}{\rho_s} \frac{\partial h_c}{\partial x} + T_s \left(\frac{\rho_s - \rho_c}{\rho_c} \right) \frac{\partial z_{ic}}{\partial x} \right] + \frac{\partial}{\partial y} \left[T_s \frac{\rho_c}{\rho_s} \frac{\partial h_c}{\partial y} + T_s \left(\frac{\rho_s - \rho_c}{\rho_c} \right) \frac{\partial z_{ic}}{\partial y} \right] - q_l \quad (6)$$

where

- h_c – CO₂ heads
- z_{ic} – brine - CO₂ interface
- z_t – elevation of the top of the reservoir
- ϕ – porosity
- q_c – injection rate of CO₂ into aquifer
- q_l – aquifer leakance across a confining bed
- S_r – residual water saturation
- S_s – brine specific storage ($S_s \sim \rho_s g \beta$)
- β – reservoir compressibility
- ρ_c – density of CO₂
- ρ_s – density of brine phase

Our sharp-interface approach assumes brine and supercritical CO₂ flow occurs only in the horizontal direction. While CO₂ density changes considerably with pressure and temperature (Nordbotten et al. 2005), our model assumed that fluid properties were spatially invariant. Our analysis considers changes in CO₂ storage due to changes in saturation and compressibility effects although the later is relatively small in comparison. Our analysis neglects diffusion of CO₂ into the brine phase (Lu and Lichtner, 2007) and fluid-rock geochemical reactions which may be significant on geologic time scales.

The head of CO₂ presented in equations (5-6) is given by:

$$h_c = \frac{P}{\rho_c g} + z \quad (7)$$

where

- P – CO₂ fluid pressure
- g – gravity constant

362 z – elevation
363

364 The head of the brine phase (h_s) is explicitly related to the head of CO₂ as follows:

365

366
$$h_s = \frac{\rho_c}{\rho_s} h_c + \frac{\rho_s - \rho_c}{\rho_s} z_{ic} \quad (8)$$

367

368 Due to the assumed coarse grain sized of the reservoir rocks, capillary forces are neglected in
369 equations (7-8). We calculate the rate of brine leakance across the Eau Claire using a one-dimensional
370 expression of Darcy's Law:

371
$$q_l = -\frac{K_z}{b'} (h_s - h_o) \quad (9)$$

372

373 where

374 K_z – vertical hydraulic conductivity of the brine phase within the confining unit
375 h_o – is the head above the confining unit
376 h_s – is (complete)
377 b' is the thickness of the confining unit
378

379 Our approach also neglects transient storage changes on flow within the confining unit. If the CO₂ lens
380 thickness at the top of the reservoir exceeds 1 m, we reduce the vertical hydraulic conductivity of the
381 confining unit by three orders of magnitude to minimize leakage in regions where CO₂ is present at
382 the top of the reservoir. We do not consider separate phase CO₂ migration across the Eau Claire
383 Formation. The transmissivities for the CO₂ and brine phases is defined as:

384

385
$$\begin{aligned} T_c &= K_c [z_T - z_{ic}] \\ T_s &= K_s [z_{ic} - z_b] \end{aligned} \quad (10)$$

386

387 where

388 K_s and K_c – vertically-averaged saturated hydraulic conductivities of the brine and CO₂ fluid
 389 phases ($K_i = k\rho_i g/\mu_i$; where i refers to the respective fluid phase;
 390 T_c and T_s - transmissivities for the CO₂ and brine phases.
 391 z_{ic} – CO₂-brine interface
 392 z_T – top of aquifer
 393 z_b – base of aquifer
 394

395 If the computed interface falls below the bottom of the reservoir, a maximum saturated thickness
 396 based on the total formation thickness is assigned in determining the reservoir transmissivity. We
 397 reduced the porosity by a factor of 100 in elements where the interface reached the bottom of the
 398 Mount Simon to minimize mass balance errors and promote lateral spreading of the CO₂-brine
 399 interface (Ledoux et al. 1990). We also maintain a minimum saturated thickness for each fluid phase
 400 (5% of total thickness) to permit the lateral movement of pressure and the CO₂ phase.

401

402 Equations 5-6 provide an accurate estimate of heads and interface near the injection wells where the
 403 CO₂ lens is non-zero. However, they don't provide an accurate prediction of far-field brine heads (h_s)
 404 because the CO₂ phase is zero away from the injection well. To overcome this limitation, we adopted
 405 the approach of Gasda (2008) and also solve a single, transmissivity based flow equation for brine
 406 head (h_s) summing CO₂ and brine transmissivity and storativity:

407

$$408 \quad \frac{\partial}{\partial x} \left[(T_s + T_c) \frac{\partial h_s}{\partial x} \right] + \frac{\partial}{\partial y} \left[(T_s + T_c) \frac{\partial h_s}{\partial y} \right] = [(z_T - z_{ic})S_c + (z_{ic} - z_b)S_s] \frac{\partial h_s}{\partial t} \quad (11)$$

409 where

410 S_s – brine specific storage coefficient

411

412 The saturated thickness of the CO₂ phase is defined by the elevations of the sharp-interface position
 413 and reservoir thickness.

414

415

416

3.3 Numerical Methods

We solved the above system of equations (5-6, 11) using the finite element method (Taylor and Person, 1996, Person et al. 1998). We solved equations 5-6 simultaneously given that there are two unknowns in each equation (h_c , z_{ic}). Equation 11 was solved separately using the freshwater and CO₂ lens thicknesses computed in equations 5-6. We solved the two sharp interface equations (5-6) simultaneously using Gaussian elimination. We then solved for brine head in equation 11 using the saturated thickness determined from equations 5 and 6. We validated our model using PFLOTRAN/FEHM for a single well injection as described below.

3.4 Boundary and Initial Conditions

For the basin scale model we specified a constant head and CO₂ lens thickness of zero along the northern edge of our solution domain. All other boundaries were no flow. For intermediate scale models, the same boundary and initial conditions were enforced.

3.5 Hubbert CO₂ Potential

The simplifying assumptions described above prevent us from computing the long-range migration pathways CO₂ due to buoyancy and hydrodynamic effects. We quantified long-range separate-phase CO₂ migration away from injection wells due to buoyancy (i.e. bed slope) and due to regional groundwater flow patterns using the approach of Hubbert (1953). Hubbert's oil potential has been used to assess the relative effects of groundwater flow on petroleum migration and entrapment in a number of petroleum basins around the world including the Williston Basin (Berg et al. 1994), Alberta Basin (Bekele et al. 2002), Illinois Basin (Bethke et al. 1991), and Paris Basins (Bekele et al. 1997). Following Hubbert's approach, we assume here that buoyancy driven supercritical CO₂ migration within porous, permeable reservoir rocks, is controlled primarily by the slope of the top of the reservoir as well as the density contrast between supercritical CO₂ and formation waters:

$$\eta_c = \frac{\rho_w}{\rho_c} Z_{ls} - \frac{\rho_w - \rho_c}{\rho_c} z_t \quad (12)$$

444

445 where η_c is Hubbert's CO₂ heads, h is hydraulic head within the Mount Simon, ρ_s is brine density, ρ_c
 446 is oil density, z_t is the elevation of the top of the reservoir. We explicitly computed the lateral CO₂
 447 migration rates as follows:

448

$$\begin{aligned} q_x &= -\frac{K_c}{\phi} \frac{\partial \eta_c}{\partial x} \\ q_y &= -\frac{K_c}{\phi} \frac{\partial \eta_c}{\partial y} \end{aligned} \quad (13)$$

450

451 where K_c is the CO₂ conductivity and q_x , and q_y are the components of CO₂ velocities in the x- and y-
 452 directions. We used the velocity field from equation (15) to produce particle streak lines of long-range
 453 CO₂ migration across the Illinois Basin.

454

455 3.6 Model Verification

456 We attempted to verify in part, our sharp-interface model, in part, by attempting to reproduce a simple
 457 a numerical injection experiment carried out using PFLOTTRAN (Lu and Lichtner, 2007) and FEHM
 458 (Pawar, 2007). These codes include equations of state for CO₂ and brine phases, relative permeability,
 459 and residual saturation effects. Supercritical CO₂ was injected into a reservoir at a rate of 2.3 kg/s (370
 460 m³/day assuming a density of 748 kg/m³) for a period of ten years. The hydrostatic pressure at the top
 461 of the 63 meter thick reservoir was set as 20 MPa (depth of 2 km). No vertical leakage was permitted.
 462 The PFLOTTRAN and FEHM solutions domain extended 1000 m away for the injection well. The
 463 PFLOTTRAN/FEHM grid had a constant vertical cell dimension of 2 meters and used 32 rows of
 464 elements. It employed a uniform grid with a lateral dimension of 2 m (i.e. Cartesian grid). The
 465 permeability and porosity of the reservoir was set at 10 mD (10⁻¹⁴ m²) and 0.15, respectively. We used

a telescoping finite element grid consisting of 2,847 nodes with a cell size varying from 5 m to 30 m. We used a water and CO₂ viscosity of 0.001 and 0.00007 Pa-s, respectively.

PFLOTTRAN/FEHM computed pressures (Fig. 13B) had to be vertically averaged and converted to CO₂ heads to compare to Sharp-CO₂ (Fig. 13D). The CO₂-brine interface was inferred to be located near the 0.5 CO₂ saturation (Fig. 13A). Near the well bore, the maximum excess head computed by PFLOTTRAN was about 150 m while the CO₂ head from our sharp-interface model was about 230 m. Both codes predicted a linear variation in head out beyond the region of CO₂ saturation (Fig. 13D). The computed position of the CO₂-brine interface in all the three models, compared favorably. The CO₂ lens was restricted to the narrow region around the well and the pressure pulse propagated out much further.

4. Results

4.1 Single-Phase Analytic Injection Models

We begin our analysis with the analytical solution of Hantush and Jacob (1955) presented in Section 3.1. We assigned a storage value (0.05) based on the compressibility of CO₂. Supercritical CO₂ compressibility (e.g. 1.43E-07 Pa⁻¹ at 38 °C and 1064 m depth) is several orders of magnitude higher than water compressibility (4.5E-10 Pa⁻¹) but is on the same order of magnitude of sediment compressibility of unconsolidated sands (Freeze and Cherry, 1979). Since there is significant uncertainty in the permeability of the Mount Simon aquifer and Eau Claire confining units we varied their values between 5-125 mD and 0.0001-0.01 mD, respectively (Table 1). The pumping rate we used is the same as is used later in our basin scale sharp-interface models.

We used a CO₂ injection rate of 10⁵ m³/year. Run 1 represents what we consider the most typical parameters for the Mount Simon (50 mD) and Eau Claire (0.001 mD) confining unit (Fig. 14A). The computed peak deviatoric pressure was about 2.5MPa (Fig. 14A). The leading edge of the pressure disturbance propagated out to about 18 km after 100 years of continuous injection. The rate of

advance of the CO₂ pressure front decreased through time from 130 m/year after 10 years of injection to about 60 m/year after 100 years. Lowering the permeability of the Eau Claire by one order of magnitude (0.0001 mD; Run 2, Table 1; Fig. 14B) and increasing the Mount Simon permeability by to 125 mD pushed the leading edge of the pressure disturbance out to about 20 km after 70 years. Deviatoric pressures within the Mount Simon aquifer increased to about 18 MPa. Lowering the permeability of the Mount Simon to 5 mD and increasing the permeability of the Eau Claire to 0.01 mD (Run 3, Table 1; Fig. 14C) resulted in the highest heads (25 MPa) but yielded the smallest radius of pressure disturbance (about 6 km after 100 years of continuous injection). Unlike the study of Birkholzer et al. (2007) these analytical solutions suggest that CO₂ injection within the Mount Simon will result in a finite radius of pressure disturbance from the injection point, which in most cases will be contained within a well field, on the order of about 20 km. If other wells are located within a radial distance of 6-20 km, there will be significant well-well interference. At a depth of 1.5 km, the excess pressure generated by our analysis was about 50% of the lithostatic pressure. Using the parameters and injection rates (2.75×10^4 m³/year) of Birkholzer et al. (2007) (Fig. 14D), produced a pressure envelop on the order of 200km and a pressure anomaly at the well head of 2.2 MPa. These values are closer to what their TOUGH2 model predicted (3 MPa or 30 Bars).

Intermediate- to Basin-Scale Sharp-Interface Models of Illinois Basin

We constructed one basin-scale (Figure 15A) and two intermediate-scale (Figures 15B-C), finite-element models of the Mount Simon-Eau Claire reservoir-confining unit across much of the Illinois Basin using the sharp-interface approach. The basin scale model domain is wedge shaped with a length of 600 km to the northwest direction and has a width which varied between 260 to 510 km in the southeast-northwest direction (Fig. 15A). Fluid and rock properties used in our model are listed in Table 2. To the south, the basin-scale model terminates near the Rough Creek Fault System at the margin of the basin where the reservoir becomes deep and thin as to be less effectual. To the north, the model terminates about 50 km south of Chicago where the groundwater within pore spaces of the Mount Simon is still saline (>50,000 ppm TDS). The two intermediate (64 by 47 km and 50 by 70

km) models (Fig. 15B-C) were also constructed to study well-well interference patterns and CO₂ lens geometry at a higher spatial resolution. The basin-scale finite element mesh is comprised of 8,160 nodes and 16,122 elements (Fig. 15A). The two intermediate scale grids were composed of between 8,081 and 9,077 nodes and 16,058 and 18,042 elements (Fig. 15B-C). The intermediate scale models are located in the middle and deep sections of the Illinois basin. This was done to evaluate the impacts of permeability and porosity trends with depth on computed excess pressures and CO₂-brine interface positions using a more highly resolved grid.

We allowed thickness, permeability, and porosity to vary spatially across the basin (Fig. 1B). The Eau Claire confining unit varies in thickness from north to south from 61 to 152m.

We allowed the Mount Simon reservoir permeability to decrease in a linear fashion from 125 mD to 10 mD from north to south. Porosity also decreases from 15% to 5% from north to south. The thickness and elevation of the Mount Simon sandstone varies from north to south from less than 150 to 610 m (Fig. 6). The maximum thickness of the Mount Simon occurs near the northern edge of the Illinois Basin (Fig. 6).

4.2 Sharp-Interface Model Results

We represented the effects of CO₂ injection from 42 power plants in our model using 726 injection wells. These wells were spaced in radial patterns between 2-4 km from the power plant sites (Fig.1C). Some wells were removed if they were located within 1 km of another injection well from an adjacent power plant. Preliminary models that used between 1-12 injection wells per power plant to emplace the 80 million metric tons of CO₂ per year resulted in simulated pore pressures that exceeded lithostatic pressures in some locations.

We injected continuously for a period of 100 years. We then shut the wells in for 100 years to determine the long-term fate of pore pressures and CO₂ lens position. Computed deviatoric pressures after 100 years were highest (up to 16.4 MPa in Fig. 16A, 17A) in the deepest part of the basin where

permeability is lowest (about 5 mD). In the middle of the basin at intermediate depths (permeability about 50mD), excess pressures reached only about 4.4 MPa (Fig 16A, 17C) after 100 years. The maximum radial distance of pressure disturbance (>0.03 MPa or 3m of freshwater head) away from individual injection wells was on the order of 9-13 km across the basin. The wells were shut in after 100 years of injection. After 200 years (100 years of shutin) fluid pressures dissipated and the region of pressure disturbance increased out to radial distances of about 15-30 km (Figs. 16B, 17B and 17D). Maximum fluid pressures decreased to between 3.6 to 9.8 MPa at intermediate and deep portions of the Illinois Basin. The net diameter of the pressure disturbance envelop around the injection well centers was about 50 km and there is significant well-well pressure disturbance between adjacent injection well centers. Intermediate scale simulations provide higher resolution images of pressure disturbance patterns. After 100 years of shutin it is difficult to see the positions of individual wells at all depths (Fig. 17B, D). However, note that the pressures will never return to hydrostatic conditions due to buoyancy effects.

The thickness and geometry of the computed CO₂ lens shows important differences across the basin (Fig. 18). Because the Mount Simon is thinnest (only 50m thick) and of low porosity (0.05) in the deepest, southern most part of the basin, the CO₂-brine interface reaches the base of the formation before displacing brines laterally (Fig. 18a). At intermediate depths, the CO₂ lens doesn't reach the base of the Mount Simon and attains a maximum thickness of 60 m. At intermediate depths, it spreads further laterally due to the increased Mount Simon permeability and porosity (Fig. 18C). The radius of the CO₂ plume varies between the deep and intermediate parts of the basin between about 0.5-2.0 km depending on local porosity levels. There is little well-well interference between individual CO₂ lenses after 100 years. After 100 years of shutin, the CO₂ lens has spread considerably at intermediate depths (Fig. 18D). The CO₂ lens lateral migration is much less in the deepest part of the basin (Fig. 18B). The maximum thickness of the CO₂ lens at intermediate depth is only 12 m after 100 years of

shutin. The CO₂ lens footprint is still much smaller when compared to the region pressure disturbance (compare Figures 17 and 18 after 100 years of shutin).

Simulated vertical leakage of brines across the Eau Claire confining units was highest (10⁻⁵ m/day; Fig 19C-D) around the injection wells just beyond the CO₂ lens terminates and dissipated quickly. After 100 years brines would have moved about 0.5 meters into the Eau Claire formation. Brine displacement was negligible at a radial distance of about 5 km from an injection well (Fig. 19A). This is due, in part, to leakage represented across the Eau Claire confining unit. Our analysis suggests there will be very limited brine displacement at the basin-scale.

To assess the potential that CO₂ injection could induce earthquakes, we plotted pore pressure verses depth for the two intermediate scale models. These show that pore pressures exceed hydrostatic pressures in the deepest part of the basin (Figure 20) but are close to hydrostatic at intermediate depths. Fluid pressures reach 46% of lithostatic pressure between 3000-3500 m depth. We also plotted pore pressures generated at the two hazardous waste injection wells near Lake Erie reported by Nicholson and Wesson, (1988, 11 MPa, open circle). This value is far below lithostatic levels.

One potential effect of increased fluid pressures is uplift of the land surface. We estimated the amount of uplift within the Mount Simon by using the following relation:

$$\Delta L = b \Delta P \alpha_{ul} \quad (15)$$

where ΔL is the amount of uplift (m), ΔP is the deviatoric pore pressure (Pa), b is the local thickness of the Mount Simon formation (m) and α_{ul} is the unloading compressibility. The compressibility (8.0x10⁻⁹ Pa⁻¹) we used is relatively low for sandstones (Freeze and Cherry, 1979) and is intended to represent unloading conditions (Corbet and Bethke, 1992). We used pore pressures presented in Figure 16 to compute uplift. Local Mount Simon thickness was used. Results indicate that up to 6 m

of uplift would occur assuming the unloading compressibility used (Figure 21). The magnitude of uplift was similar for the intermediate and deep portions of the basin due to the offsetting effect of decreasing Mount Simon formation thickness with increasing pore pressure to the south.

4.3 Long-Range CO₂ Migration Due to Buoyancy and Hydrodynamic Drives

Our sharp-interface models were unable to represent the effects of long-range separate phase CO₂ migration because of the underlying assumptions described above (i.e. a constant elevation assigned to the Mount Simon Formation and no regional head gradients). However, using Hubbert (1953) (equations 12-13) potential theory, we were able to estimate the rate of separate phase CO₂ migration. We found that separate phase migration would be induced primarily due to the effects of buoyancy (bed slope). The buoyant drive is low due to the gentle slope on the Mount Simon from North to South (about 0.008 m/m). However the hydrodynamic drive is even less due to the low hydraulic gradients within the Mount Simon (Fig. 8A; about 0.0008 m/m). Our analysis suggests that separate phase CO₂ within the deepest portion of the basin would migrate up gradient to the north before becoming entrapped within gentle structures in the middle of the basin (Fig. 21). The migration rates are small (6 m/1000 years) and it is likely that much of the CO₂ would either diffuse into the water phase, be trapped in the capillary pore spaces, or become fixed in the reservoir as a solid mineral phase on these time scales (Rubin et al., 2005).

5. Discussion and Conclusions

We had originally suspected that the injection of 80 million metric tons of CO₂ per year over a period of 100 years at 41 sites would lead to significant displacement of brines towards the margins of the basin and basin scale pressure anomalies. However, because of leakage of brine across the Eau Claire confining unit and the distributed nature of power plant locations across the States of Illinois and Indiana, our models indicated that long-range (> 20 km) lateral movement of brines and pressure anomalies will not develop. That said, the model predicts that pressures in excess of 16.4 MPa would occur in the deepest parts of the basin and pressure interference patterns would emerge between

adjacent injection wells in the more permeable center of the basin. Our calculated maximum pressure anomaly was about 5 times higher than that predicted by simulations using TOUGH2 (Birkholzer et al. 2007; 3 MPa). However, our computed pressure anomalies were restricted to a distance of about 13 km from injection wells in our sharp-interface models. Since the analytical results presented in Figure 14, were able to nearly match Birkholzer et al. 2007 and our sharp interface results, we suspect that these differences are mostly due to the differences in selection of petrophysical parameters (1000 mD for Birkholzer et al. 2007 verses 125 mD for this study) rather than differences in model assumptions. One of the biggest surprises of our study is how well simple analytic solutions can approximate the results of more complex multiphase simulations.

Significant anomalous pressures due to CO₂ injection only developed in the deepest part of the Illinois Basin where the permeability is lowest (Fig. 16D). While excess pressures were about 46 % of the lithostatic load, they would have been much higher if fewer wells had been used. Relatively low deviatoric pressure conditions to the north suggest that the middle portion of the Illinois Basin is probably the best venue for injection. This is especially true if one considers seismic hazards which are concentrated to the south. If CO₂ transmission costs are not prohibitive, then power utilities should consider focusing on the middle of the Illinois Basin for long-term injection programs.

Long range CO₂ migration by buoyancy or hydrodynamics does not appear to be an important concern. Salinity changes induced by brine migration into low porosity confining units are capable of producing significant osmotic pressures up to 20 MPa (Neuzil, 2000) if significant concentration gradients develop. This could lead to unanticipated consequences such as hydrofracturing. While vertical brine leakage rates are low, the presence of abandon wells may still be a factor (Nordbotten et al. 2004, 2005) in CO₂ leakage. If CO₂ remains in a separate phase over geologic time scales, buoyancy effects would cause it to travel at a rate of 6 m/1000 years to the north. The effects of groundwater flow on CO₂ migration are small due to the gentle head gradients.

Our basin-scale model was able to represent 200 years of CO₂ injection, migration, and pore pressure development at the sedimentary basin scale using serial computer. Equivalent two-phase simulations representing 30 years of injection required the use of high performance computing. While our sharp interface model is relatively simple (e.g. we only consider one reservoir and one confining unit), it could be used to perform first cut assessments of optimal location and type (horizontal verse vertical) of CO₂ injection wells across the Illinois Basin. It serves as an end member, a worst case scenario, in the set of linked analyses that must ultimately consider the effects of dissolution into the brine, capillary entrapment and mineral precipitation in the overall performance of fluid migration in a basin. If a system of pure piston-like displacement has such minimal effects on pressure and brine migration, when other mitigating factors as itemized above are integrated, the migration scenarios should be even less distinct. More work could also be done in the Illinois Basin extending our analysis to multiple formation targets for CO₂ injection (e.g. the Knox carbonate section, New Albany Shale and Pennsylvanian coals) and calibrating our model to match available pressure (Gupta and Bair, 1999) and salinity data. This would involve linking multiple sharp-interface reservoirs/confining unit models together at the basin scale.

6. References

- Athy, L.F., 1930. Density, porosity, and compaction of sedimentary rocks. American Association of Petroleum Geologists Bulletin. 14, 1-23.
- Beaumont, C., Quinlan, G., Hamilton, J., 1988. Orogeny and stratigraphy: numerical models of the Paleozoic in the eastern interior of North America. Tectonics. 7, 389-416.
- Bethke, C.M., Reed, J.D., Oltz, D.F., 1991. Long-range petroleum migration in the Illinois Basin. American Association of Petroleum Geologists Bulletin. 75, 925-945.
- Berg, R.R., DeMis, W.D., Mitsdarffer, A. R., 1994. Hydrodynamic effects on Mission Canyon (Mississippian) oil accumulations, Billings Nose area, North Dakota. American Association of Petroleum Geologists Bulletin. 78, 508-518.
- Beleke, E., Person, M.A., Rostron, B.J., Barnes, R., 2002. Modeling secondary oil migration with core-scale data: Viking Formation, Alberta Basin. American Association of Petroleum Geologists Bulletin. 86, 55-74.
- Beleke, E., Person, M., de Marsily, G., 1997. Petroleum migration pathways and charge concentration; a three-dimensional model; discussion. American Association of Petroleum Geologists Bulletin. 83, 1015-1019.
- Birkholzer, J., Zhou, Q., Zhang, k., Jordan, P., Rutqvist, J., Tsang, C.F., 2007. Large-Scale Hydrological Evaluation and Modeling of the Impact on Groundwater Systems, NETL Project Annual Report, October 1, 2007.
- Bredehoeft, J.D., Blyth, C.R., White, W.A., Maxey, G.B., 1963. Possible mechanism for concentration of brines in subsurface formations. Bulletin of the American Association of Petroleum Geologists. 47, 257-269.
- Breemer, C.W., Clark, P.U., Haggerty, R., 2002. Modeling the subglacial hydrology of the late Pleistocene Lake Michigan Lobe, Laurentide Ice Sheet. Geological Society of America Bulletin. 114, 665-674.
- Chadwick, R.A., Zweigel, P., Gregersen, U., Kirby, G.A., Holloway, S., Johannesen, P.N., 2003. Geological characterization of CO₂ storage sites: Lessons from Sleipner, northern North Sea.

695 Proceedings of the 6th International Conference on Greenhouse Gas Control Technologies
 696 (GHGT-6), J. Gale and Y. Kaya (eds.), 1–4 October 2002, Kyoto, Japan, Pergamon, v.I, 321–
 697 326
 698 Clauser, C., 1992. Permeability of crystalline rocks. EOS, Transactions American Geophysical Union.
 699 73, 233-240.
 700 Cramer, C.H., Wheeler, R.L., Mueller, C.S., 1992. Analysis for seismic hazard in the southern Illinois
 701 Basin. Seismological Research Letters. 73, 792-805.
 702 Corbet, T., Bethke, C.M., 1992. Disequilibrium fluid pressures and groundwater flow in the Western
 703 Canada sedimentary basins. Journal of Geophysical Research. 97, 7203-7217.
 704
 705 Eager, K., Pavlis, G., Hamberger, M., 2006. Evidence of Possible Induced Seismicity in the Wabash
 706 Valley Seismic Zone from Improved Microearthquake Locations. Bulletin of the Seismological
 707 Society of America. 96, 1718–1728.
 708 Freeze, R.A., Cherry, J.A., 1979. Groundwater. 604 pp., Prentice-Hall, New Jersey.
 709 Gasda, S.E., 2008. Numerical Models for Evaluating CO₂ Storage in Deep, Saline Aquifers: Leaky
 710 Wells and Large-Scale Geological Features, Ph.D. Dissertation, Princeton University.
 711 Gasda, S.E., Nordbotten, J.M., Celia, M.A., 2008. Upslope Plume Migration and Implications for
 712 Geological CO₂ Sequestration in Deep Saline Aquifers. IES Journal A: Civil and Structural
 713 Engineering. 1, 2-16.
 714 Gupta, N., Bair, E.S., 1997. Variable-Density Flow in the Midcontinent Basins and Arches Region of
 715 the United States. Water Resources Research. 33, 1785–1802.
 716 Hanor, J. S., Origin and Migration of Subsurface Sedimentary Brines, SEPM Short Course No. 21,
 717 247 pp., Society of Economic Paleontologists and Mineralogists, Tulsa, OK, 1987.
 718 Hanor, J., McIntosh, J.C., 2006. Are secular variations in seawater chemistry reflected in the
 719 compositions of basinal brines? Journal of Geochemical Exploration. 89, 153-156.
 720 Hantush, M.S., Jacob, C.E., 1955. Non-steady radial flow in an infinite leaky aquifer: American
 721 Geophysical Union Transaction. 36, 95–100.

722 Hovorka et al., 2001. Evaluation of brine-bearing sands of the Frio Formation, upper Texas Gulf
723 Coast for geological sequestration of CO₂, DOE/NETL-2001/114.

724 Hsieh, P.A., Bredehoeft, J.D., 1981. A reservoir analysis of the Denver earthquakes; a case of induced
725 seismicity. *Journal of Geophysical Research*. 86, 903-920.

726 Hubbert, M.K., 1953. Entrapment of petroleum under hydrodynamic conditions. *American*
727 *Association of Petroleum Geologists Bulletin*. 37, 1954–2026.

728 Kolata, D.R., Nelson, W.J., 1990. Tectonic History of the Illinois Basin, in Leighton, M.W., Kolata,
729 D.R., Oltz, D.F., Eidel, J.J., (editors). *Interior Cratonic Basins*. American Association of
730 *Petroleum Geologists Memoirs*. 51, 263 - 285.

731 Ledoux, E., Rivera, E., and G. de Marsily, 1990. A compatible single-phase/two-phase numerical
732 model, *Ground Water*. 28, 79-87.

733 Lehner, F.K., Marsal, D., Hermans, L., Van Kuyk, A., 1987. A model of secondary hydrocarbon
734 migration as a buoyancy-driven separate phase flow, in *Migration of Hydrocarbons in*
735 *Sedimentary Basins*, edited by B. Doligez, pp. 457-471, Editions Technip, Paris.

736 Lindholm, 1990. Effects of present and projected ground-water withdrawals on the Twin Cities
737 aquifer system, Minnesota. *US Geological Survey Water Resources Investigation 90-4001*, 129
738 p.

739 Liu, G., Zheng, C., Gorelick, S.M., 2004. Limits of applicability of the advection-dispersion model in
740 aquifers containing connected high-conductivity channels, *Water Resources Research*. 40.
741 W08308, doi:10.1029/2003WR002735.

742 Lloyd, O.B., Jr., Lyke, W.L., 1995. *Ground Water Atlas of the United States, Segment 10--Illinois,*
743 *Indiana, Kentucky, Ohio, and Tennessee: U.S. Geological Survey Hydrologic Investigations*
744 *Atlas 730-K*, 30 p.

745 Lu, C., Lichtner, P., 2007. High resolution numerical investigation on the effect of convective
746 instability on long term CO₂ storage in saline, Aquifers, *Journal of Physics: Conference Series*
747 78, 012042 doi:10.1088/1742-6596/78/1/012042.

- Medina, C., Barnes, D., Rupp, J., 2008. Depth Relationships in Porosity and Permeability in the Mount Simon Sandstone of the Midwest Region: Applications for Carbon Sequestration: Eastern Section Meeting of the American Association of Petroleum Geologists, Pittsburgh, PA.
- McIntosh, J.C., Walter, L.M., Martini, A. M., 2004. Extensive microbial modification of formation water geochemistry: Case study from a Midcontinent sedimentary basin, United States. Geological Society of America Bulletin. 116, 743-759.
- Medina, C.R., Barnes, D.A., Rupp, J.A., 2008. Depth Relationships in Porosity and Permeability in the Mount Simon Sandstone (Basal Sand) of the Midwest Region: Applications for Carbon Sequestration (Poster, AAPG-SPE Eastern Meeting, 11 - 15 October 2008, Pittsburgh, Pennsylvania).
- Neuzil, C.E., 2000. Osmotic generation of 'anomalous' fluid pressures in geological environments. Nature. 403, 182-184.
- Nicholson C., Roeloffs, E., Wesson, R.L., 1988. The Northeastern Ohio Earthquake of 31 January 1986: was it induced? Bulletin of the Seismological Society of America 78, 188-217.
- Nicholson, C., Wesson, R.L., 1990. Earthquake hazard associated with deep well injection: A report to the U.S. Environmental Protection Agency. U.S. Geological Survey Bulletin 1951, 74 pp., U.S. Geological Survey, Reston, Va.
- Nordbotten, J., Celia, M., Bachu, S., Dahle, H., 2005. Semi-analytic solution for CO₂ leakage through an abandoned well. Environmental Science and Technology. 39, 602-611.
- Nordbotten, J., Celia, M., Bachu, S., 2004. Analytical solution for leakage rates through abandoned wells. Water Resources Research. 40, WO4204.
- Nordbotten, J.M., Kavetski, D., Celia, M.A., Bachu, S., 2008. A Semi-analytical Model Estimating Leakage associated with CO₂ Storage in Large-scale Multilayered Geological Systems with Multiple Leaky Wells, published online 17th December 2008, *Environmental Science and Technology*, 2008.
- Olcott, P.G., 1992. Ground Water Atlas of the United States, Segment 9--Iowa, Michigan, Minnesota, and Wisconsin: U.S. Geological Survey Hydrologic Investigations Atlas 730-J, 31 p.

775 Obermeier, S.F., Munson, P.J., Munson, C.A., Martin, J.R., Frankel, A.D., Youd, T.L., Pond, E.C.,
 776 1992. Liquefaction evidence for strong Holocene earthquake(s) in the Wabash Valley of
 777 Indiana-Illinois. *Seismological Research Letters*. 63, 321-335.

778 Pawar, R., 2007. Multiphase Flow Simulations Of Large-Scale CO2 Sequestration Operation: How
 779 Do You Incorporate Details Of Wellbores In Coarse Grids? American Institute of Chemical
 780 Engineers, Annual Meeting, Salt Lake City, abstract 518b.

781 Person, M., Taylor, J., Dingman, S.L., 1998. Sharp-Interface Models of Salt Water Intrusion and Well
 782 Head Delineation on Nantucket Island, Massachusetts. *Ground Water*. 36, 731-742.

783 Person, M., Roy, P., Wright, H., Ito, E., Winter, T., Rosenberry, D., Gutowski, W., Cohen, D., Morin,
 784 P., 2007. Hydrologic Response of the Crow Wing Watershed, Minnesota to Mid-Holocene
 785 Climate Change. *Geological Society of America Bulletin*. 119, 363-376.

786 Person, M.A., McIntosh, J., Bense, V.F., Remenda, V., Pleistocene Hydrology of North America: The
 787 role of icesheets in reorganizing groundwater flow systems. *Reviews of Geophysics*. 45,
 788 RG3007, doi:10.1029/2006RG000206, 2007.

789 Rhea, L., Person, M., de Marsily, G., Ledoux, E., Galli, A., 1994. Geostatistical Models of Secondary
 790 Petroleum within Heterogeneous Carrier Beds: A Theoretical Example. *American Association*
 791 *of Petroleum Geologists*. 78, 1679-1691.

792 Rubin, E., Meyer, L. and H. de Coninck, 2005. IPCC Special Report on Carbon Dioxide Capture and
 793 Storage: Prepared by Working Group III of the Intergovernmental Panel on Climate Change,
 794 Intergovernmental Panel on Climate Change, Cambridge.

795 Schlegel, M., McIntosh, J., Person, M., Ballentine, C., Zheng, Z., 2008. Investigating the source and
 796 timing of freshwater recharge into saline aquifers in the glaciated Illinois Basin, *Geochimica et*
 797 *Cosmochimica Acta*. 72, A832.

798 Seeber, L., Armbruster, J.G., Kim, W.Y., 2004. A fluid-injection-triggered earthquake sequence in
 799 Ashtabula, Ohio: Implications for seismogenesis in stable continental regions. *Bulletin of the*
 800 *Seismological Society of America*. 24, 76-87.

801 Stueber, A.M., Walter, L.M., 1994. Glacial Recharge and Paleohydrologic Flow Systems in the
802 Illinois Basin - Evidence From Chemistry of Ordovician Carbonate (Galena) Formation
803 Waters. Geological Society of America Bulletin. 106, 1430-1439.

804 Taylor, J., Person, M., 1996. Capture Zone delineation on island aquifer systems. Ground Water. 36,
805 722-730.

806 Walton, W.C., 1960. Leaky artesian aquifer conditions in Illinois, Illinois State Water Survey Report
807 Investigation 39, 27 pp.

808 Walton, W. C., 1962. Future water-level declines in deep sandstone wells in Chicago Region. Ground
809 Water. 2, 13-20.

810 Wheeler, R.L., Cramer, C.H, 2002. Updated seismic hazard in the southern Illinois Basin; geological
811 and geophysical foundations for use in the 2002 USGS national seismic-hazard maps.
812 Seismological Research Letters. 73, 776-791.

813 Witherspoon, P., Neuman, S., 1967. Evaluating a lightly permeable caprock in aquifer gas storage, 1:
814 Caprock of infinite thickness. Trans. AIME. 240, 949.

815 Witherspoon, P.A., Mueller, T. D., Donovan, R.W., 1962. Evaluation of underground gas storage
816 conditions in aquifers through investigations of groundwater hydrology. Journal of Petroleum
817 Technology. 14, 555-562.

818 Zoback, M.D., Hickman, S., 1982. In-situ study of the physical mechanisms controlling induced
819 seismicity at Monticello Reservoir, South Carolina. Journal of Geophysical Research. 87,
820 6959-6974.

821 Zoback, M.D., Zoback, M.L., 1989. In situ stress, crustal strain and seismic hazard assessment in
822 eastern North America, Earthquake Hazards and the Design of Constructed Facilities in the
823 Eastern United States (K.H. Jacob & C.J. Turkstra, eds.), Annals of the New York Academy of
824 Sciences, v. 558, p. 54-65, N.Y. Acad. Sci., NY, 1989, 457 pp.

825 Zoback, M.D., Zoback, M.L., 1989. State of stress in the earth's lithosphere. In Encyclopedia of Solid
826 Earth Geophysics (D.E. James, ed.), Encyclopedia of Earth Sciences Series (R.W. Fairbridge,
827 Series Ed.), Van Nostrand Reinhold Co., New York, 1221-1232.

828 Zoback, M.D., Zoback, M.L., 1989. Tectonic stress field of the continental U.S. In Geophysical
829 Framework of the Continental United States (eds. L. Pakiser and W. Mooney), GSA Memoir,
830 172, 523-539.

831 Zoback, M.D., Harjes, H.-P., 1997. Injection induced earthquakes and crustal stress at 9 km depth at
832 the KTB deep drilling site, Germany. Journal of Geophysical Research. 102, 18,477-18,491.

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7. Figure Captions

Figure 1. (A) Location and capacity of coal fired power plants across Illinois Basin. The outline of the model domain is indicated by the red trapizoid (source: <http://www.midcarb.org>). (B) Changes in porosity, permeability and thickness of the Mount Simon and Eau Claire confining units with depth along A-A' shown in (A). (C) Illustration of injection well spacing at power plants represented in our sharp interface model.

Figure 2. (A) Locations, estimated magnitudes, and age of Holocene earthquake activity across southern Illinois Basin. Major fault systems include the Rough Creek (RC) and Lusk Creek (LC) Fault Systems. The shaded patterns denote active fault systems or seismogenic zones. Earth quake magnitudes and ages are based on scale and ^{14}C age dates of liquefaction features such as sand dikes in the vicinity of fault systems (after Wheeler and Cramer, 2002). The red circles denote the estimated earthquake magnitudes in the southern Illinois Basin. Blue lines indicated direction of maximum horizontal stress inferred from bore hole stress tests and borehole elongation data (from Nicholson and Wesson, 1990). (B) Location of earthquakes and hazardous waste injection wells in the Ohio-Pennsylvanian boarder, Mount Simon Formation. Injection of 320 L/min at a depth of 1.8 km resulted in up to 11 MPa of deviatoric pressures and are thought to have induced M2.6-M4.3 earthquakes (from Nicholson and Wesson, 1990).

Figure 3. Drawdown patterns (in meters) in Cambro-Ordovician aquifer system near Chicago (A) and in Mount Simon formation near Minneapolis/St Paul (B). Drawdrown patterns around Chicago also include Ironton galesville and Mount Simon formations (after Walton, 1960). Drawdown exceeds 183 m near Chicago and 45 m near Minneapolis/St. Paul due to municipal water well withdrawals which are on the same order of magnitude as CO_2 produced from power plants (squares in D). (C) Cumulative freshwater withdraws, Minneapolis/St Paul. (D) Basemap showing location of powerplants. Boxes show location of Figures 3A and 3B. (after Olcott, 1992; Lloyd and Lyke, 1995).

Figure 4. Plan-view (A) and cross-sectional (B) representation of Illinois basin stratigraphy. This study focuses on hydrodynamics within the basal Mount Simon aquifer and overlying Eau Claire confining unit.

Figure 5. Spatial variations in elevation of the top of the Mount Simon Formation across the Illinois Basin.

Figure 6. Spatial variations in the thickness (in meters) of Mount Simon Formation the Illinois Basin.

Figure 7. N-S cross section in western Indiana showing gamma ray curves (in red) and porosity curves (in blue). A preliminary subdivision of the Mount Simon Sandstone (orange, yellow) and overlying Eau Clair confining unit (gray) is shown based primarily on gamma logs. Our analysis focuses on the orange middle unit which exhibits highest permeability values.

Figure 8. (A) Mount Simon head and (B) salinity patterns across Illinois Basin and (C) salinity-depth profiles within Illinois Basin (Figure 8A after Gupta and Bair, 1999).

Figure 9. TOUGH2 simulation of pore pressures for Mount Simon formation resulting from injection of 390 MT/year of supercritical CO₂ using 26 wells located in the center of the Illinois Basin after a period of 30 years (after Birkholzer et al. 2007). Injection pressures reached 30 Bars (3 MPa) and propagated to basin margins (~200 km). The CO₂ was injected into a sub-member of the Mount Simon with an assigned permeability of 1000 mD. The location of the sharp interface model (Sharp_CO2) domain presented in this study is also shown.

Figure 10. Porosity-depth relationship for the Mount Simon sandstone based on core analyses of 128 wells and geophysical logs from 189 additional wells. These data indicate an (Athy type) exponential relationship exists between porosity and depth (Medina et al, 2008).

Figure 11. Porosity-Permeability data for Mount Simon Formation shows a log-linear positive relationship between porosity and permeability (Medina et al, 2008).

Figure 12. Schematic diagram depicting variables and processes represented by sharp interface model of Illinois Basin.

Figure 13. Comparison of PFLOTTRAN/FEHM (A,B) and Sharp-CO₂ (C,D) models. A single well injecting 2.3 kg/s of supercritical CO₂ into a confined aquifer for a period of 10 years is represented in this test case. Vertically averaged heads and interface positions were estimated from (A,B) and compared to sharp-interface model (C,D).

Figure 14. Analytical calculations of CO₂ injection into the Mount Simon reservoir with leakage across the overlying Eau Clair confining unit using leaky aquitard solution of Hantush and Jacob (1955). Fluid was injected at a constant rate of $2.2 \cdot 10^5 \text{ m}^3/\text{day}$ (A,B,C) and $2.75 \cdot 10^4 \text{ m}^3/\text{day}$ (D) continuously for a period of 100 years (A,B,C) and 30 years (D). The numbers on the lines (Figures 14A,B,C,D) are years since the onset of injection. Note that the horizontal axis limits of Figures 14A-C differs from Figure 14D.

Figure 15. Basin-scale (A), and intermediate-scale (B-C) finite element grids of CO₂-brine transport, Illinois Basin.

Figure 16. Basin scale simulated deviatoric fluid pressures (in MPa) after 100 years of injection (A) and 100 years of shutin (B).

Figure 17. Deviatoric pressures at deep (A) and intermediate (C) depths within the Illinois Basin after injection of 100 million metric tons of CO₂ using 726 injection wells over a 100 year period using

refined grids. Fluid pressures after 100 years of shutin (200 years) are presented in Figure 16B and 16D for deep and intermediate depths. The locations of the models are shown in Figure 16.

Figure 18. Simulated CO₂ lens thickness at (deep and intermediate) depths across the Illinois basin after 100 years of continuous injection of 80 million metric tons of CO₂ using 726 injection wells. The locations of these models are shown in Figure 16.

Figure 19. Simulated lateral brine displacement rates (A,B) and vertical (C,D) brine leakage through the Eau Claire Formation (in m/day) after 100 years of continuous injection of 80 million metric tons of CO₂ using 726 injection wells.

Figure 20. Computed fluid pressure verses depth for intermediate (1700-200 m depth) and deep (2900-3500 m depth) reservoirs. Deviatoric pressure reached about 46% of lithostatic levels in the deepest part of the basin after 100 years of continuous CO₂ injection. Also plotted (circle) is inferred pressure and depth within Mount Simon near Ashtabula, Ohio which is believed to have produced M2.6-M4.3 earthquakes between 1987-2001 as a result of 10MPa of deviatoric pressures associated with hazardous waste injection (Ashtabula, OH pore pressures are from Nicholson and Wesson, 1990).

Figure 21. Computed uplift at the land surface after 100 years of continuous CO₂ injection.

Figure 22. Plan view contour map of Hubbert CO₂ heads (in m) and separate phase CO₂ migration directions (lines with arrows) due to buoyancy and hydrodynamic effects. Stream traces indicate that most of the CO₂ would be captured in gentle structural traps at the intermediate depth within the Illinois Basin.

8. Tables

Table 1. Aquifer and Confining Unit properties used in Sensitivity Analysis

Run	UNIT	*k/k'	k (mD)	k' (mD)	⁺ b (m)	[#] b' (m)	^{\$} S
1	Mount Simon	50000	50	0.0010	500	50	0.05
1	Eau Claire		50	0.0010			
2	Mount Simon	1250000	125	0.0001	500	50	0.05
2	Eau Claire		125	0.0001			
3	Mount Simon	50	5	0.1000	500	50	0.05
3	Eau Claire		5	0.1000			

*k/k' ratio of horizontal to vertical permeability for the Mount Simon and Eau Claire

⁺ saturated thickness of the Mount Simon, [#] b' saturated thickness of the Eau Claire

^{\$}Storativity of Mount Simon assuming CO₂ dominated fluid phase

Table 2. Fluid, Rock, and Injection Well Properties used in Illinois Basin Simulations

CO ₂ Viscosity	0.004 mPa-s
CO ₂ Density	500 kg/m ³
Brine Viscosity	0.25 mPa-s
Brine Density	1,100 kg/m ³
Injection well Radius	0.15 m
Injection Well Rate	283.47 m ³ /day
S _r	0.00

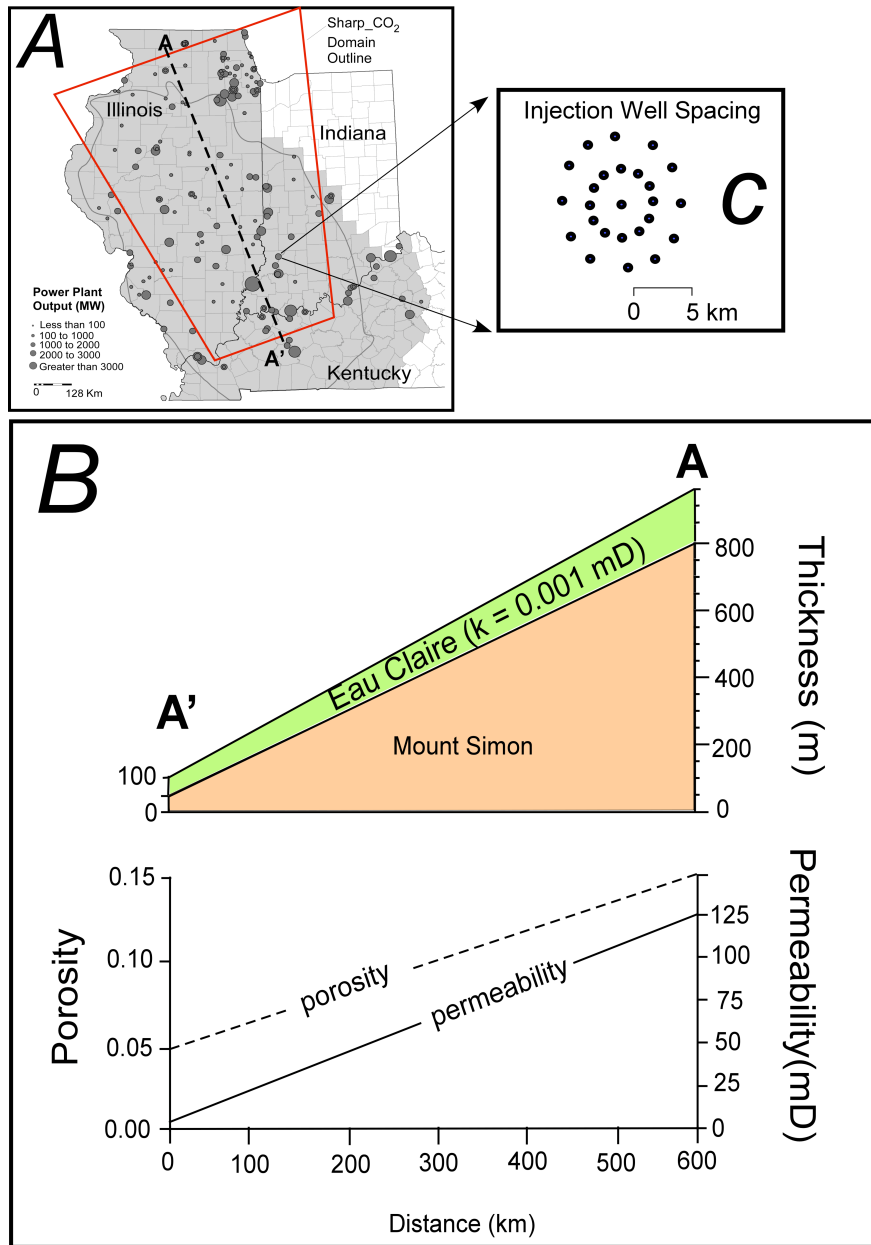


Figure 1

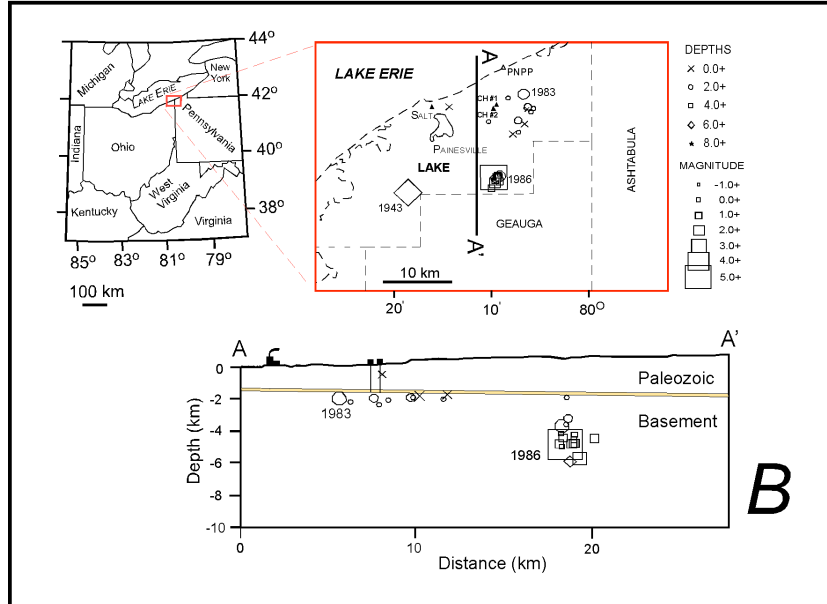
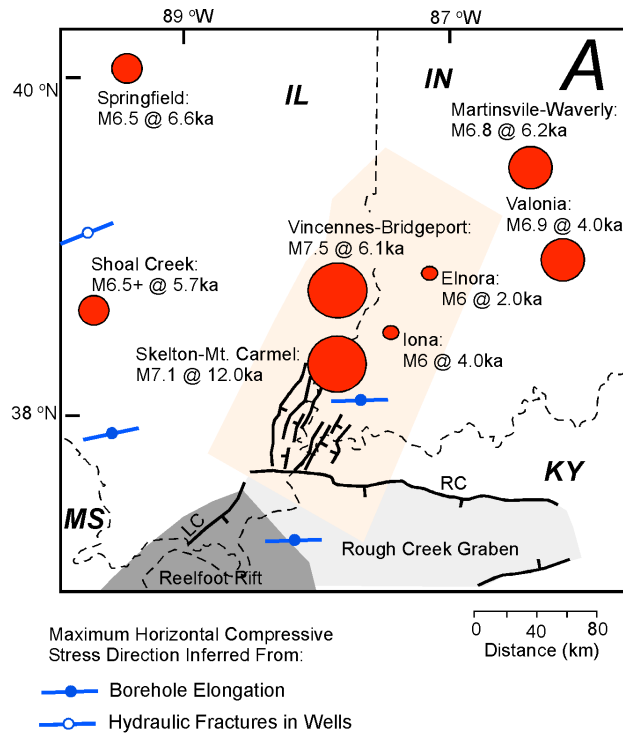


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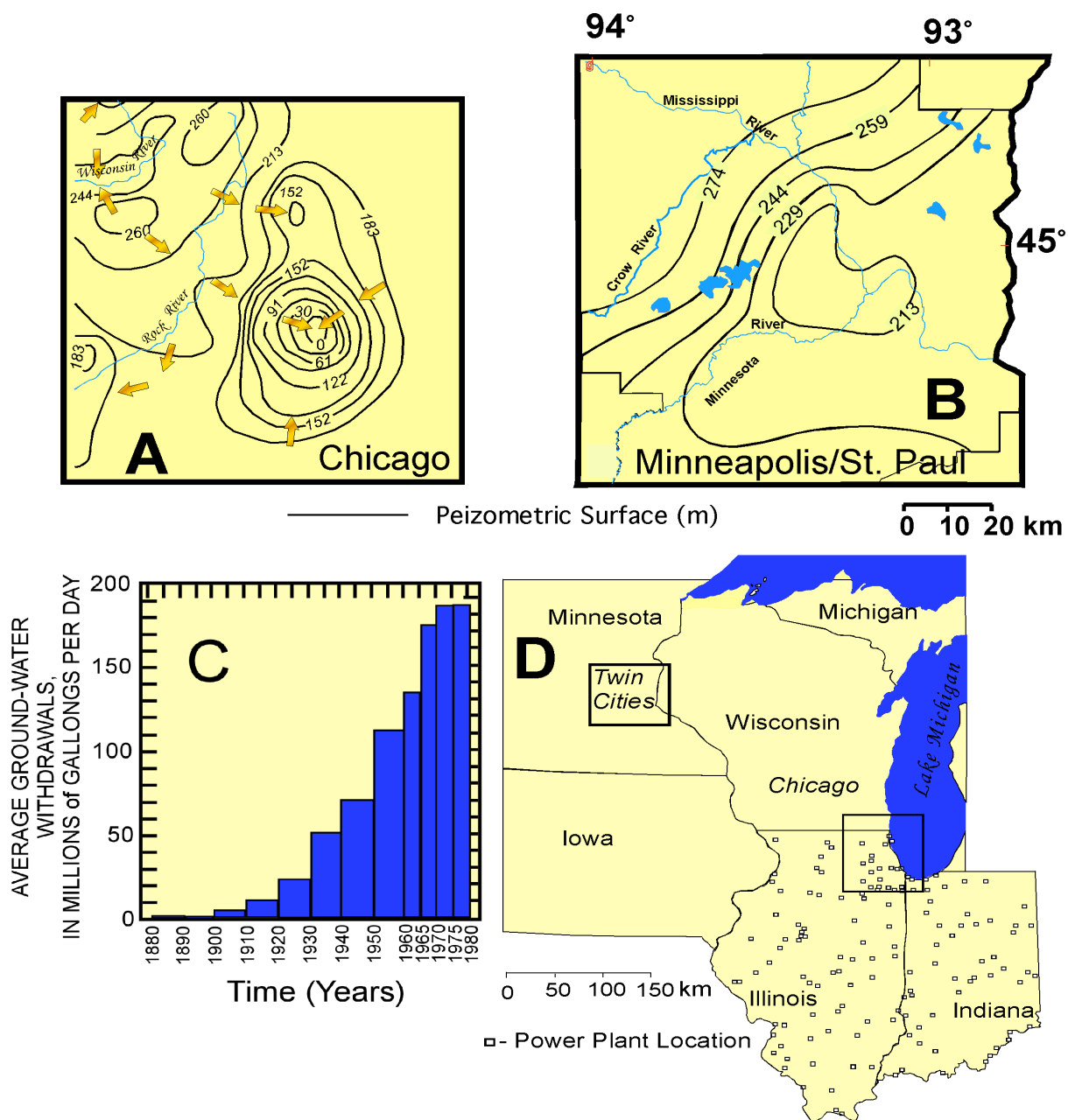


Figure 3

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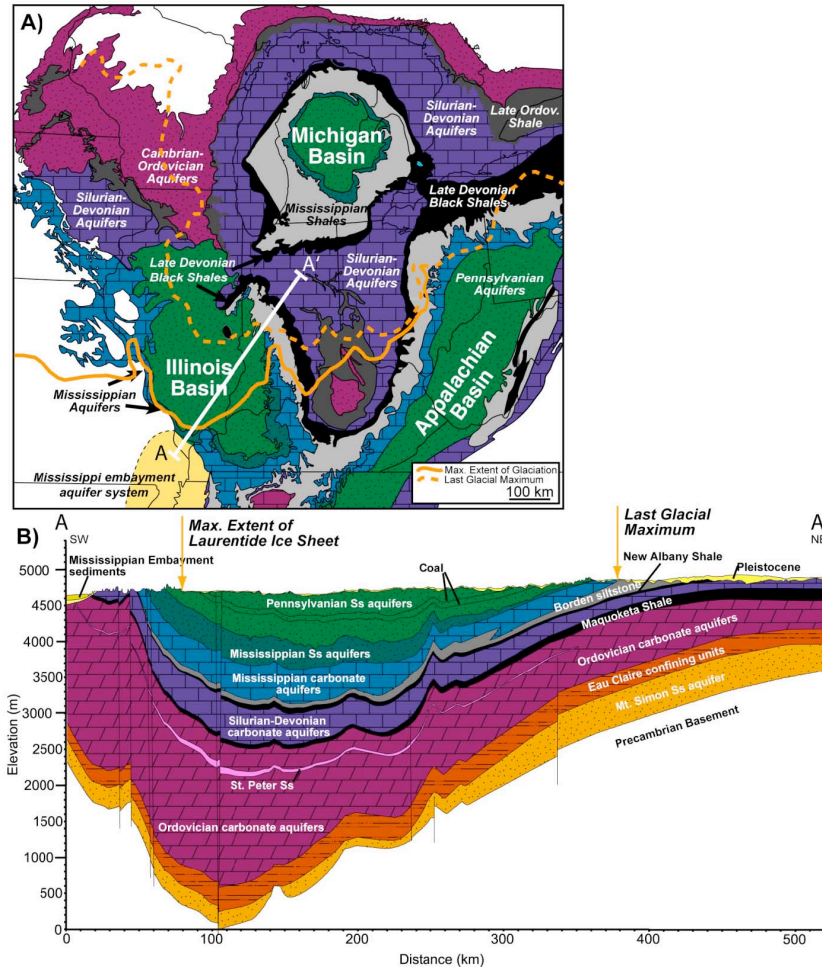


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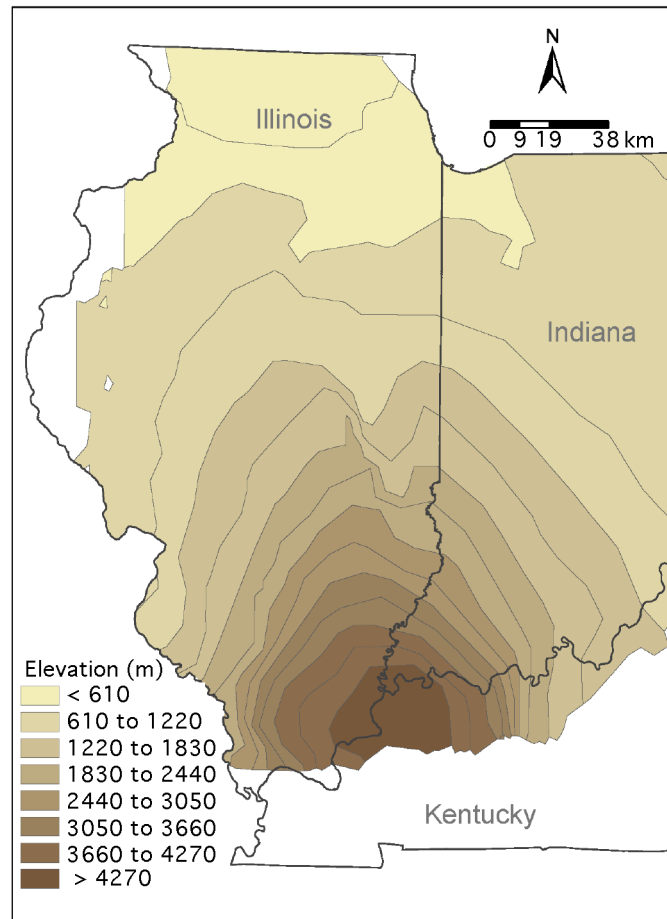


Figure 5

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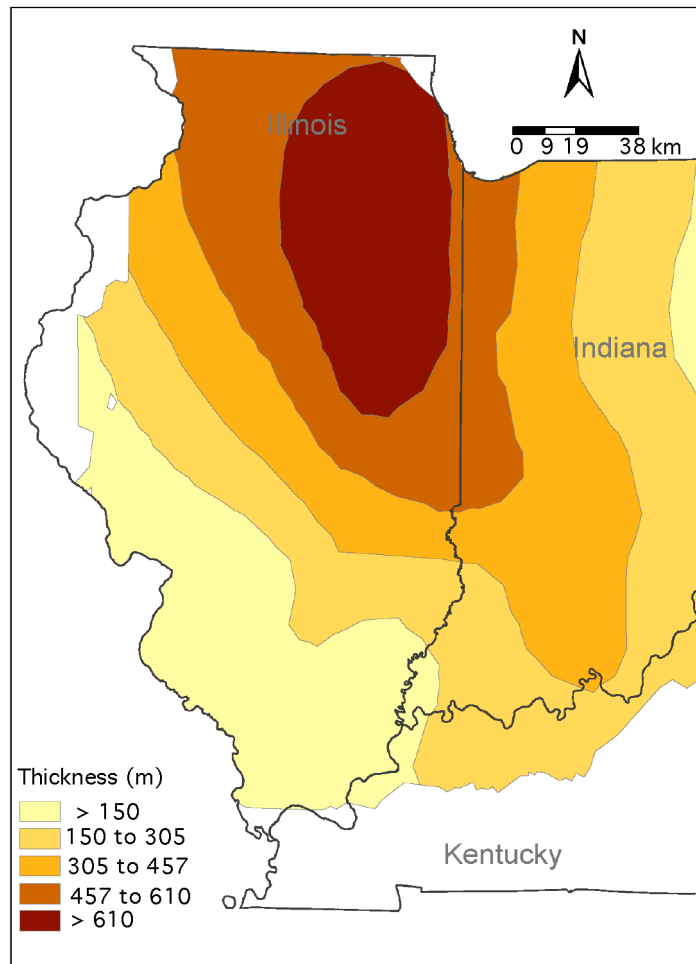


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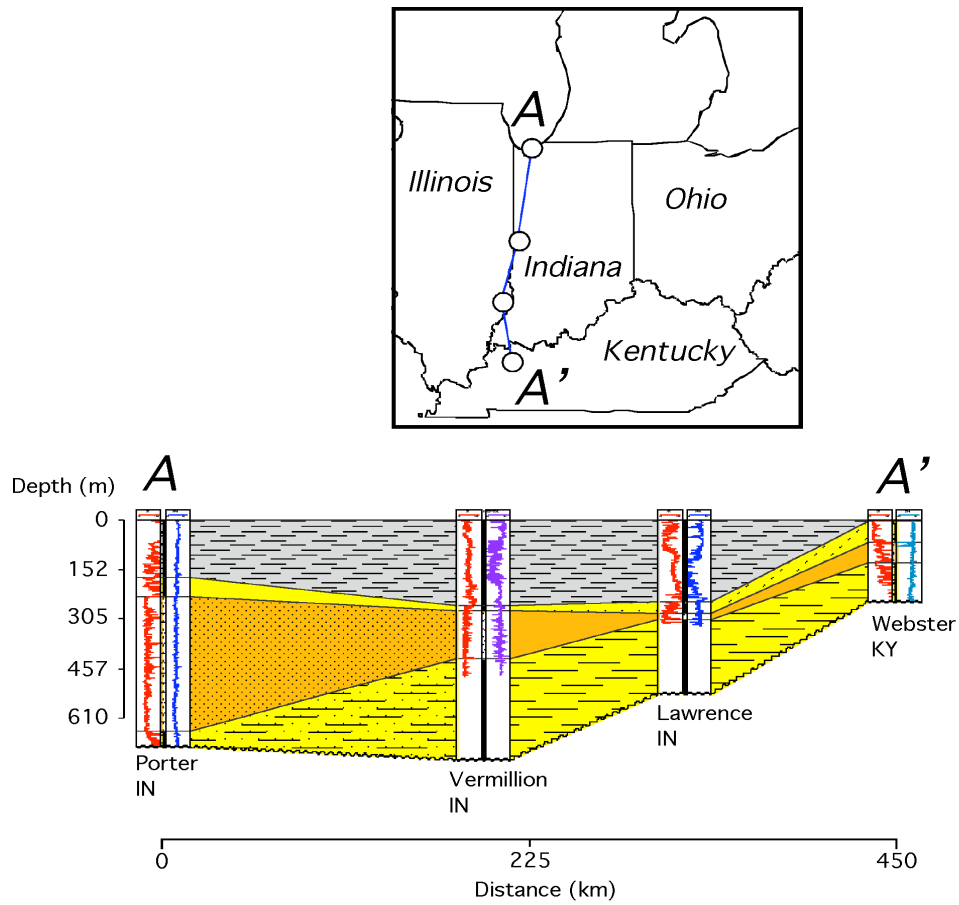


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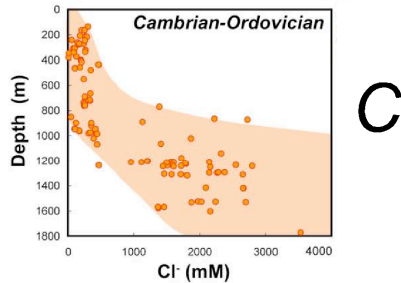
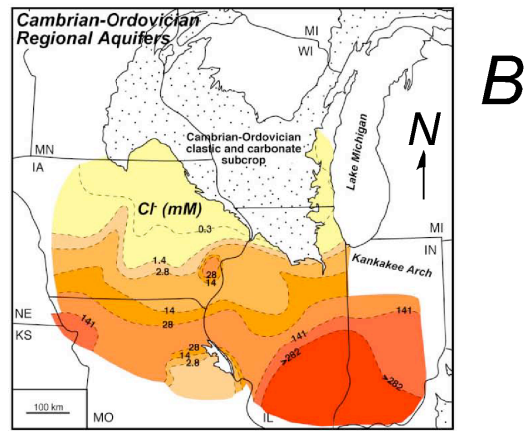
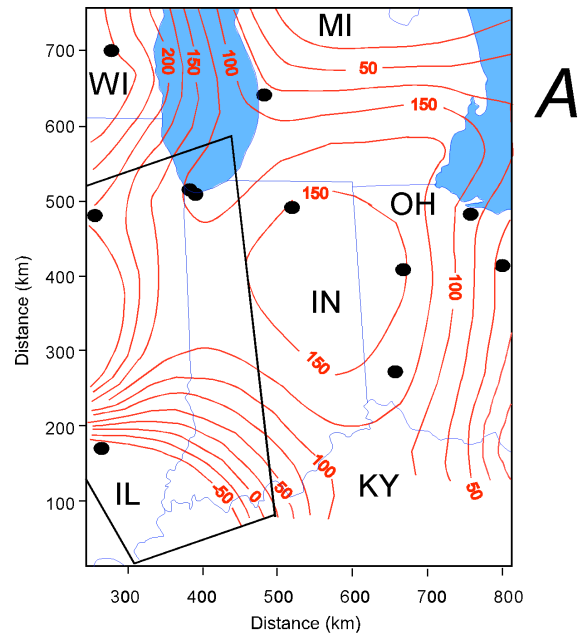
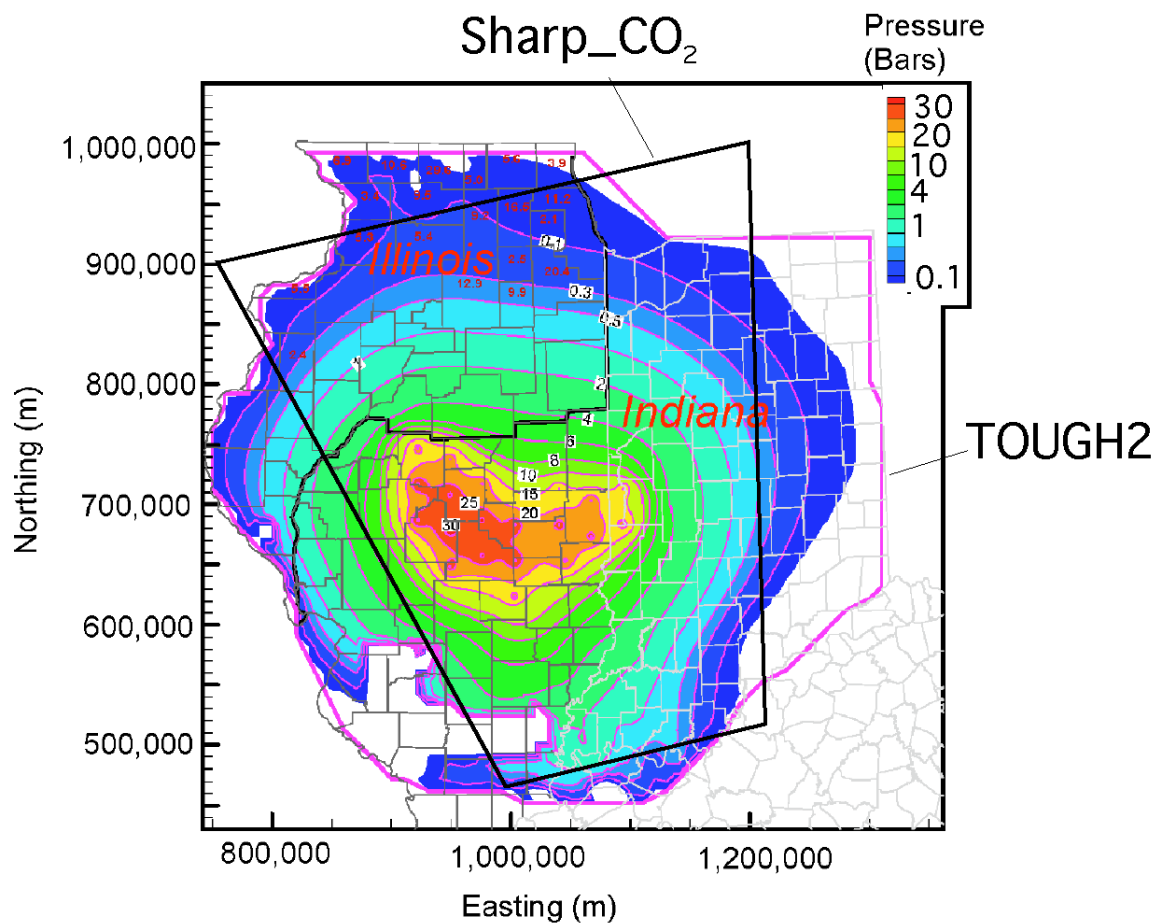


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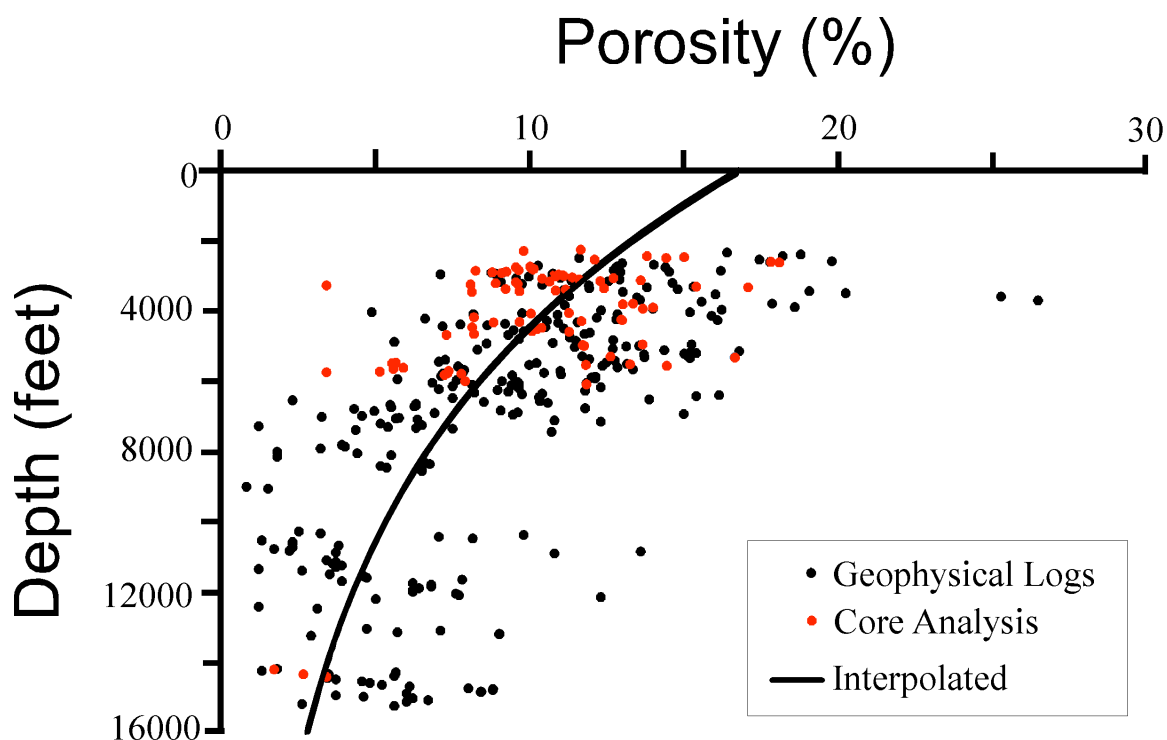
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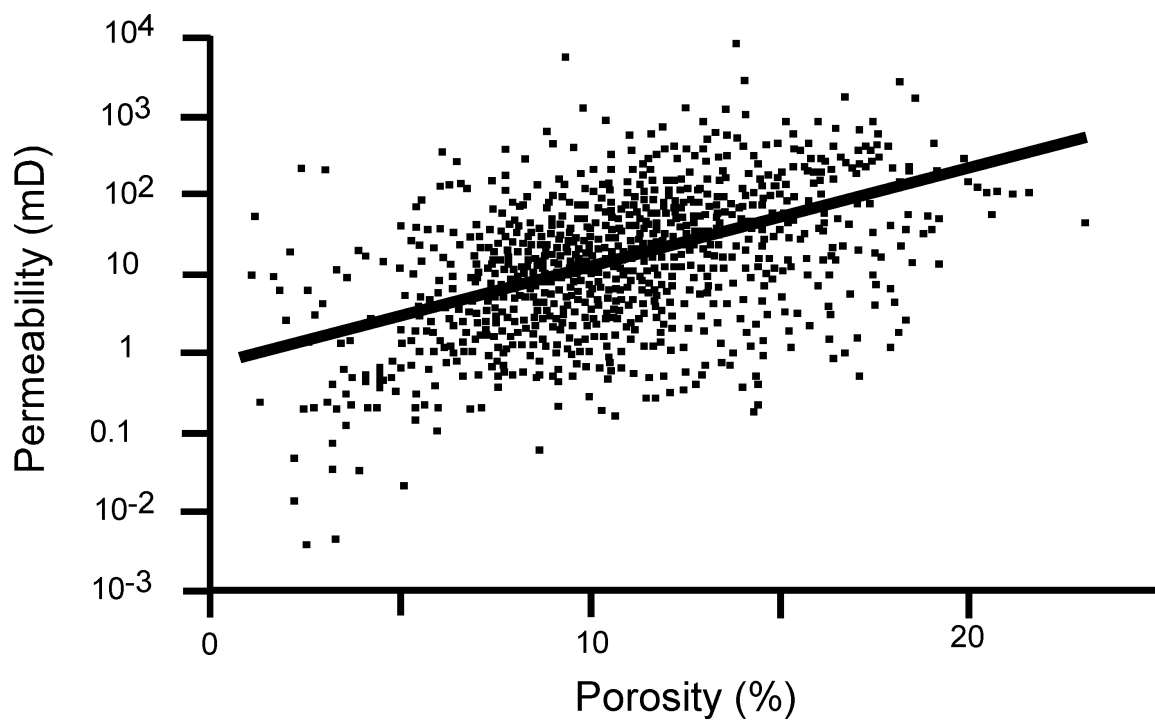
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Figure 10

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Figure 11

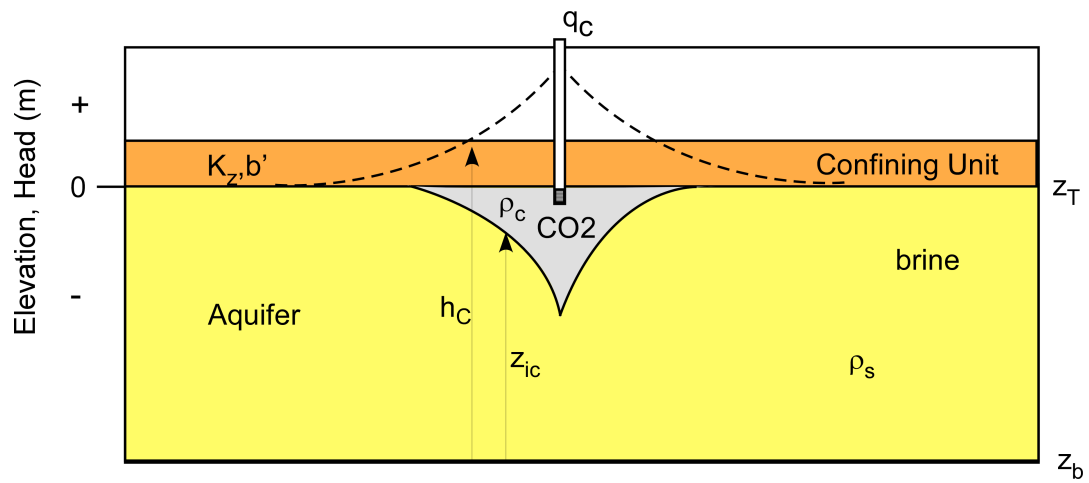


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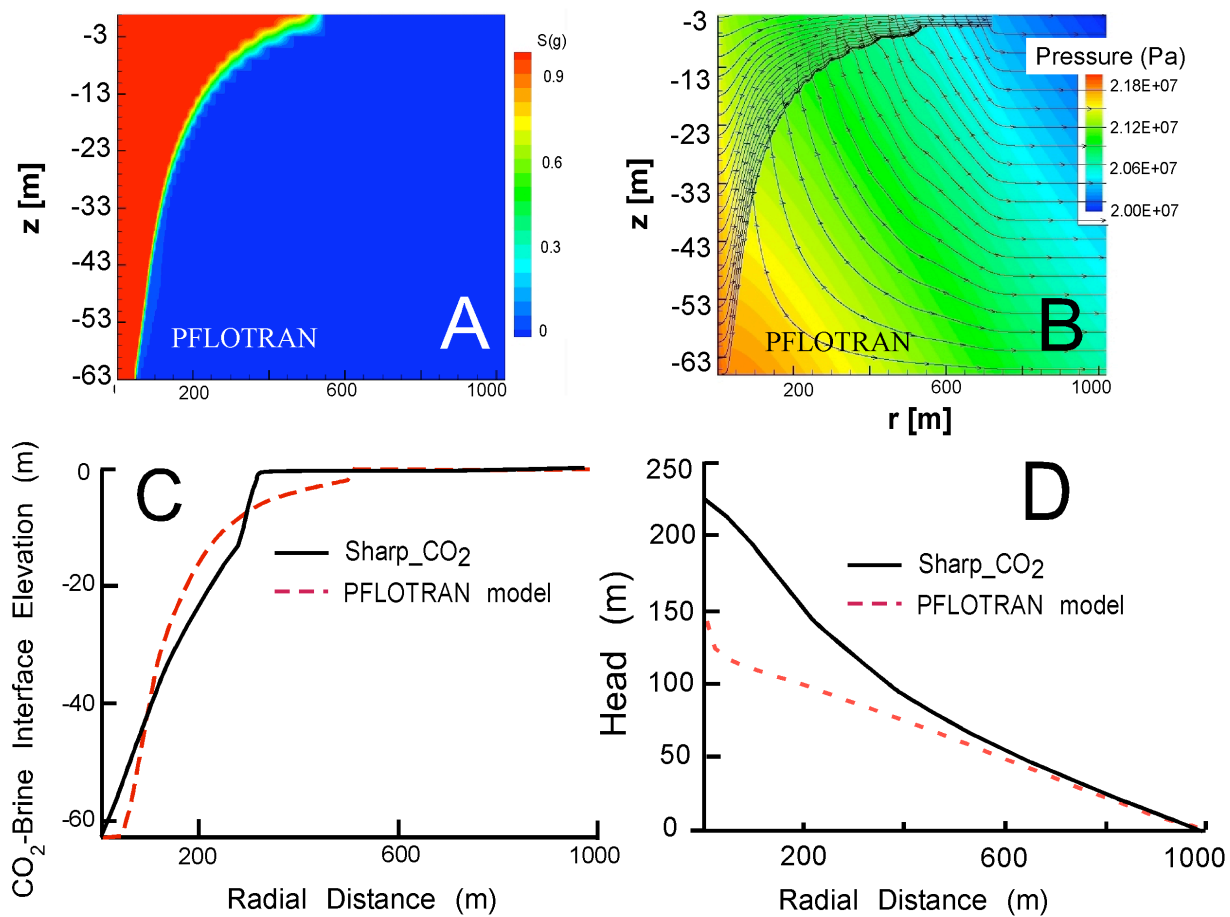
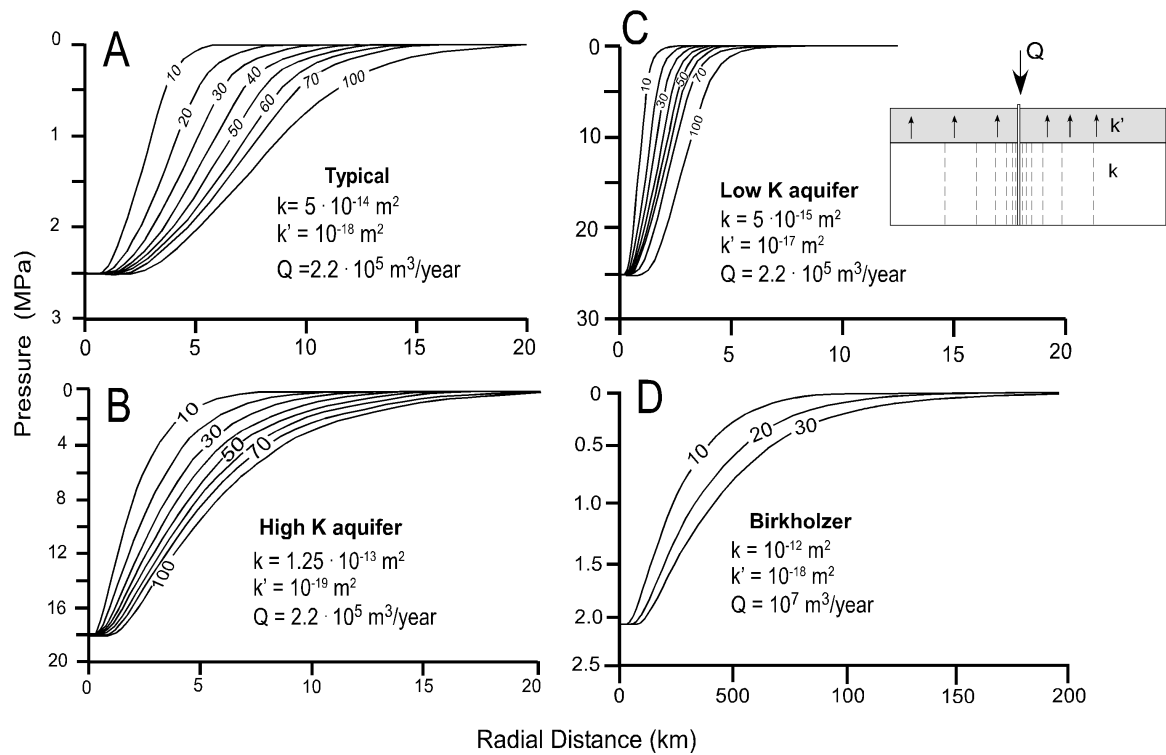


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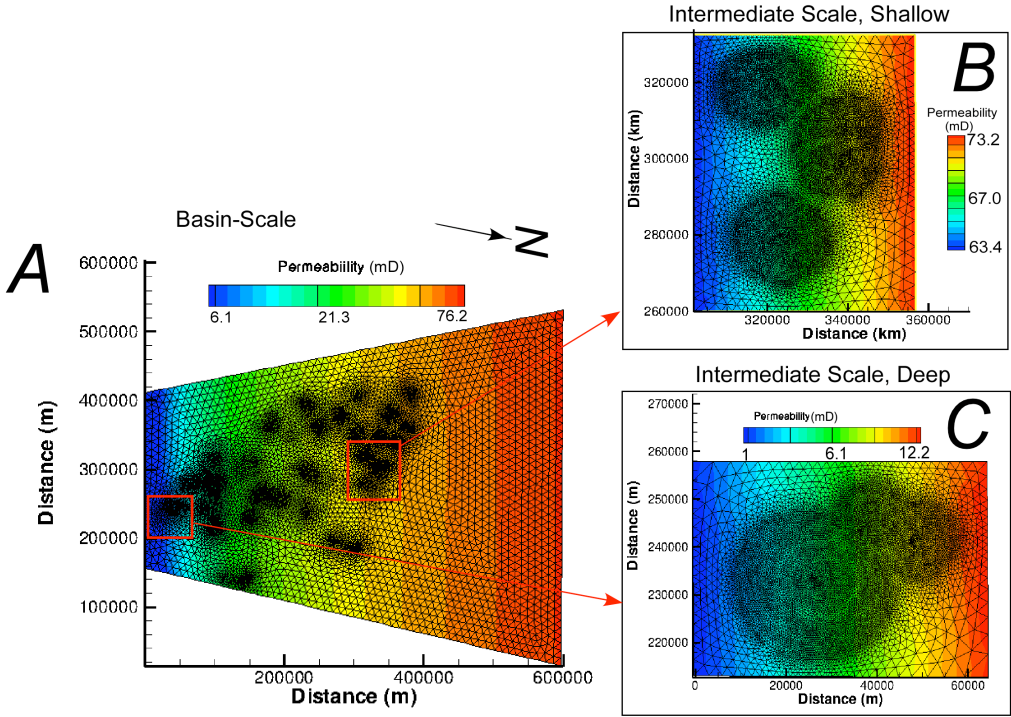
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Figure 14

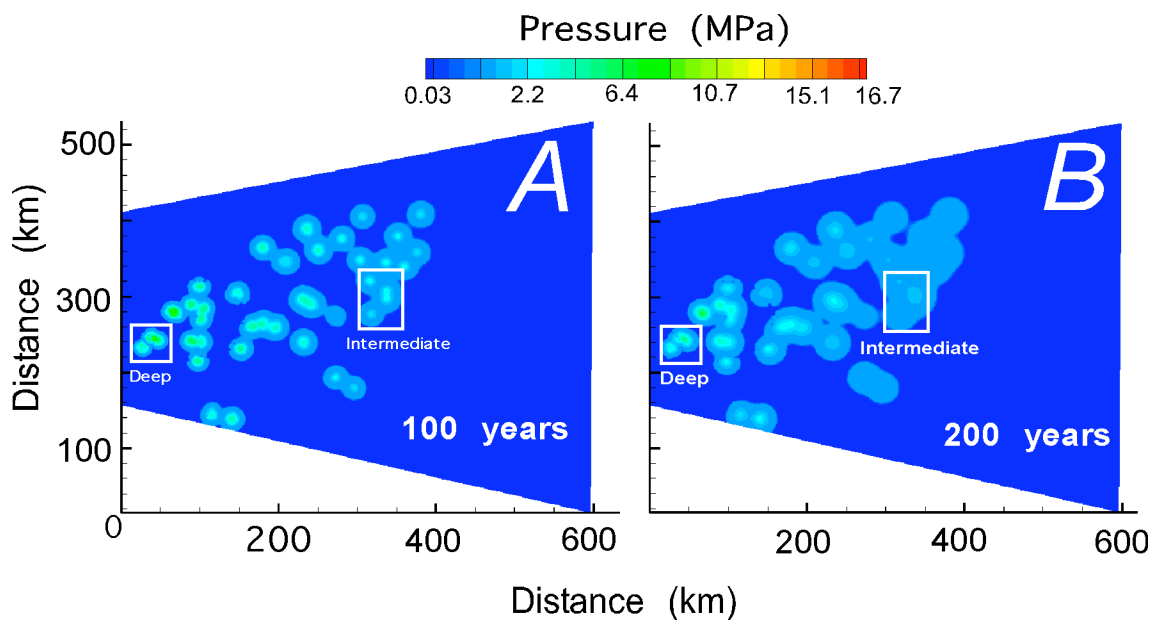
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Figure 15

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Figure 16

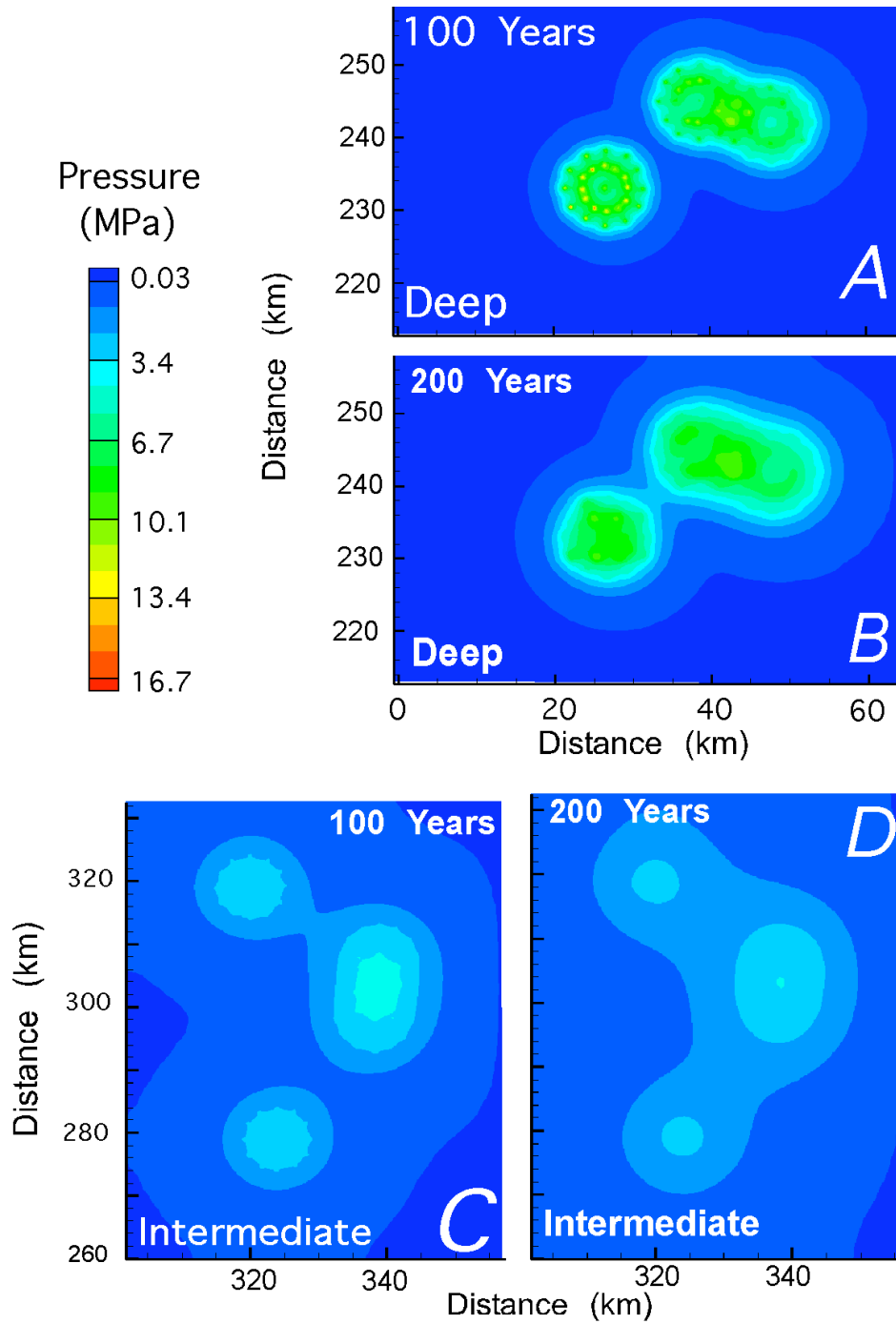
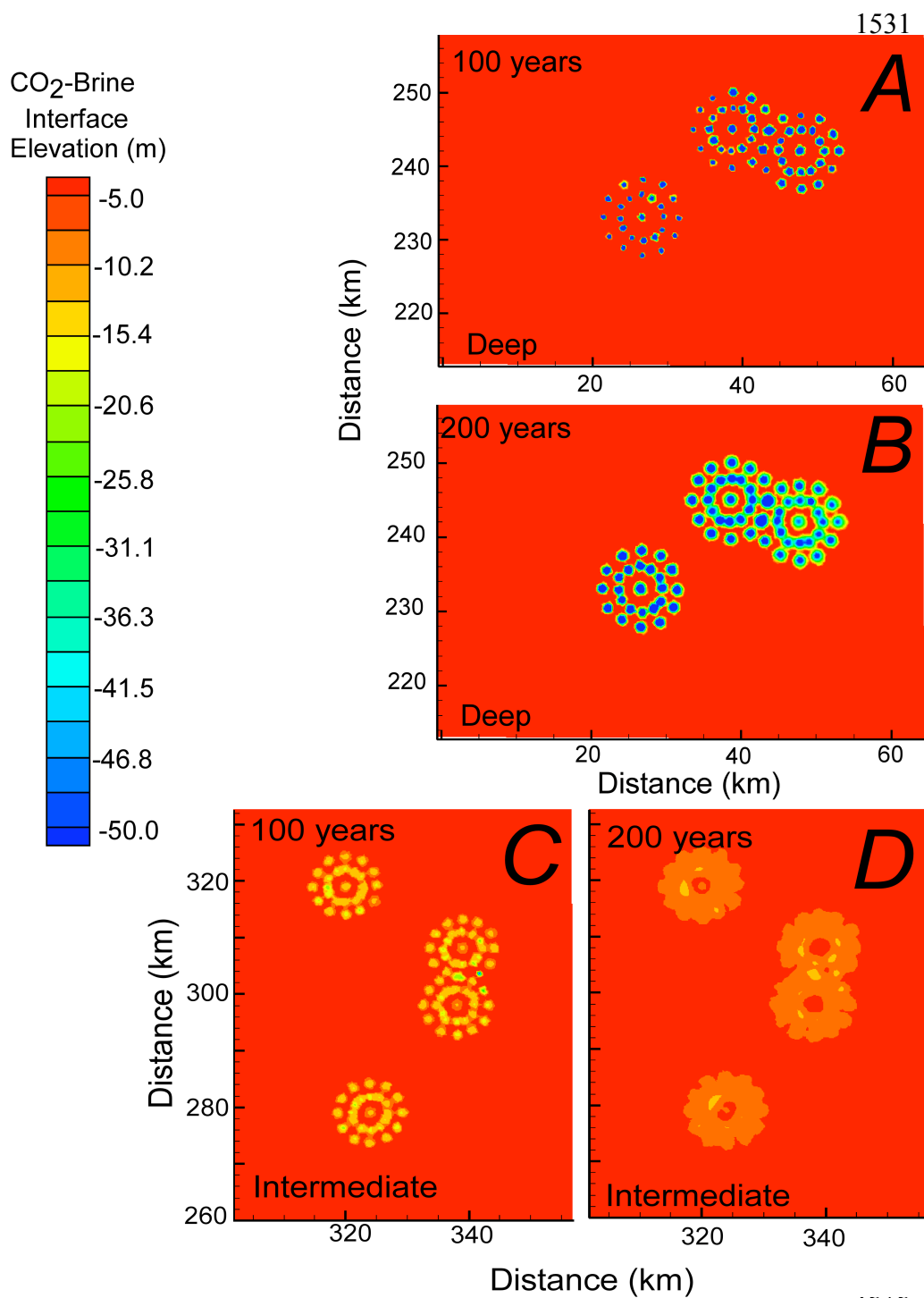


Figure 17

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Figure 18

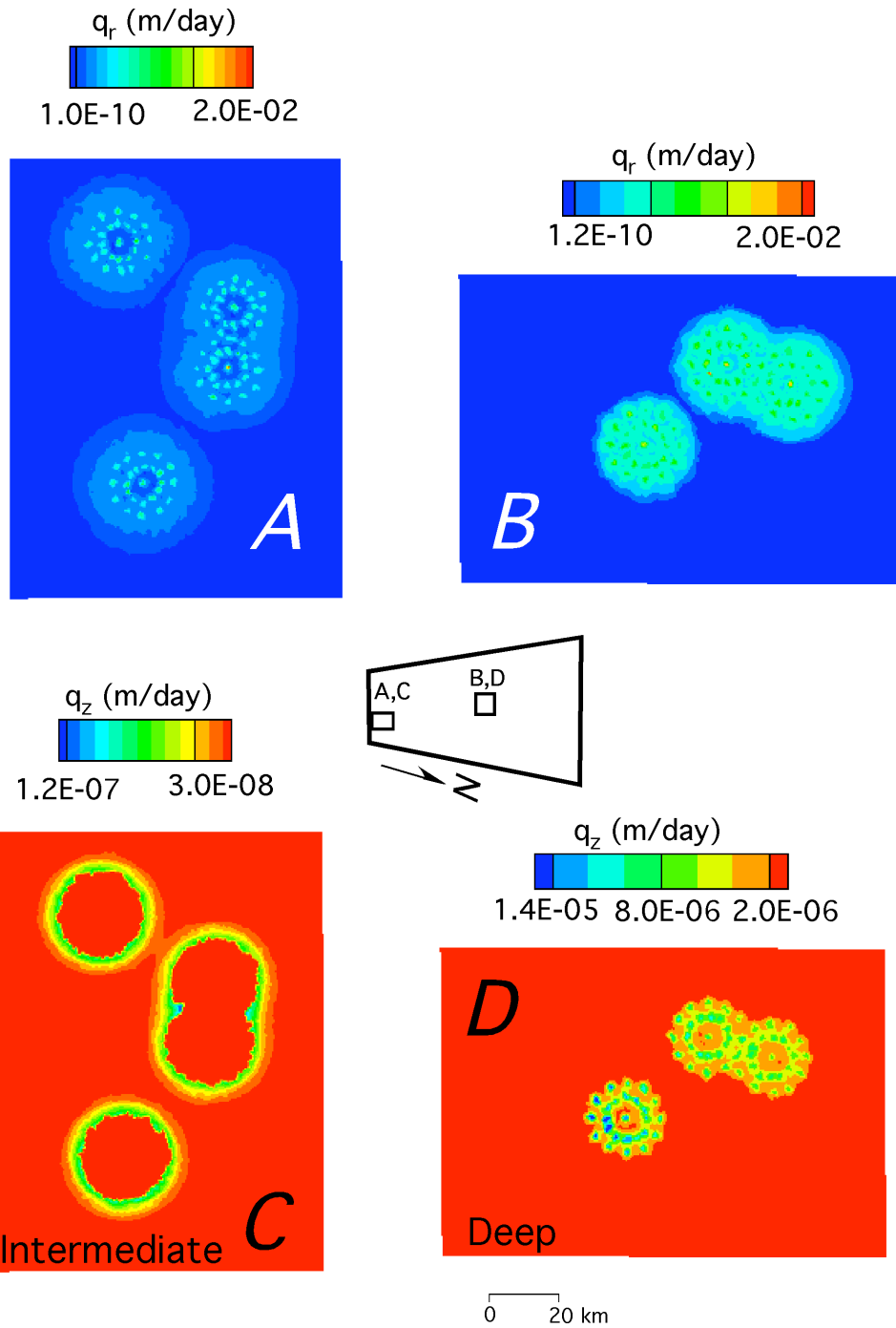
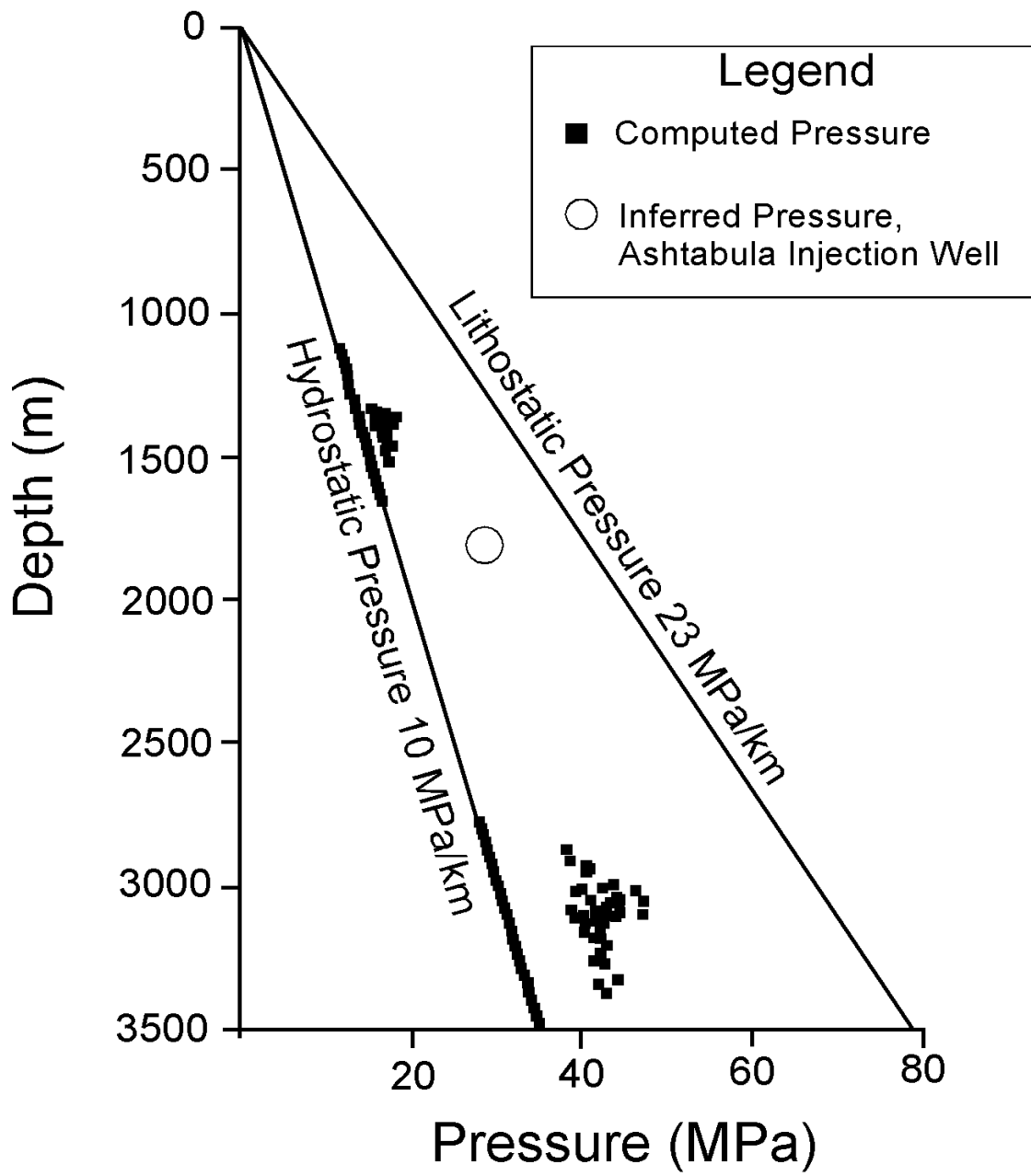


Figure 19

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Figure 20

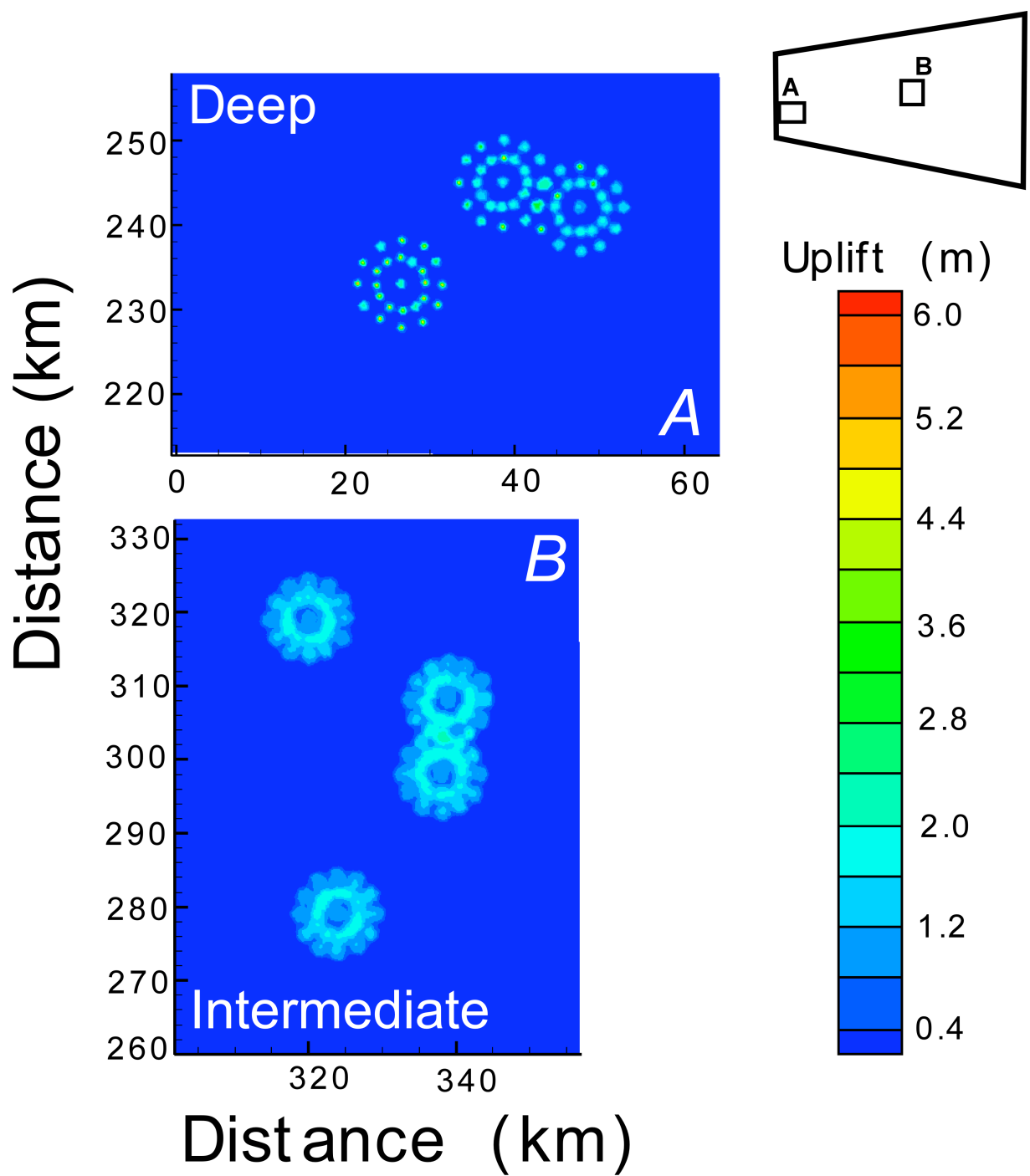
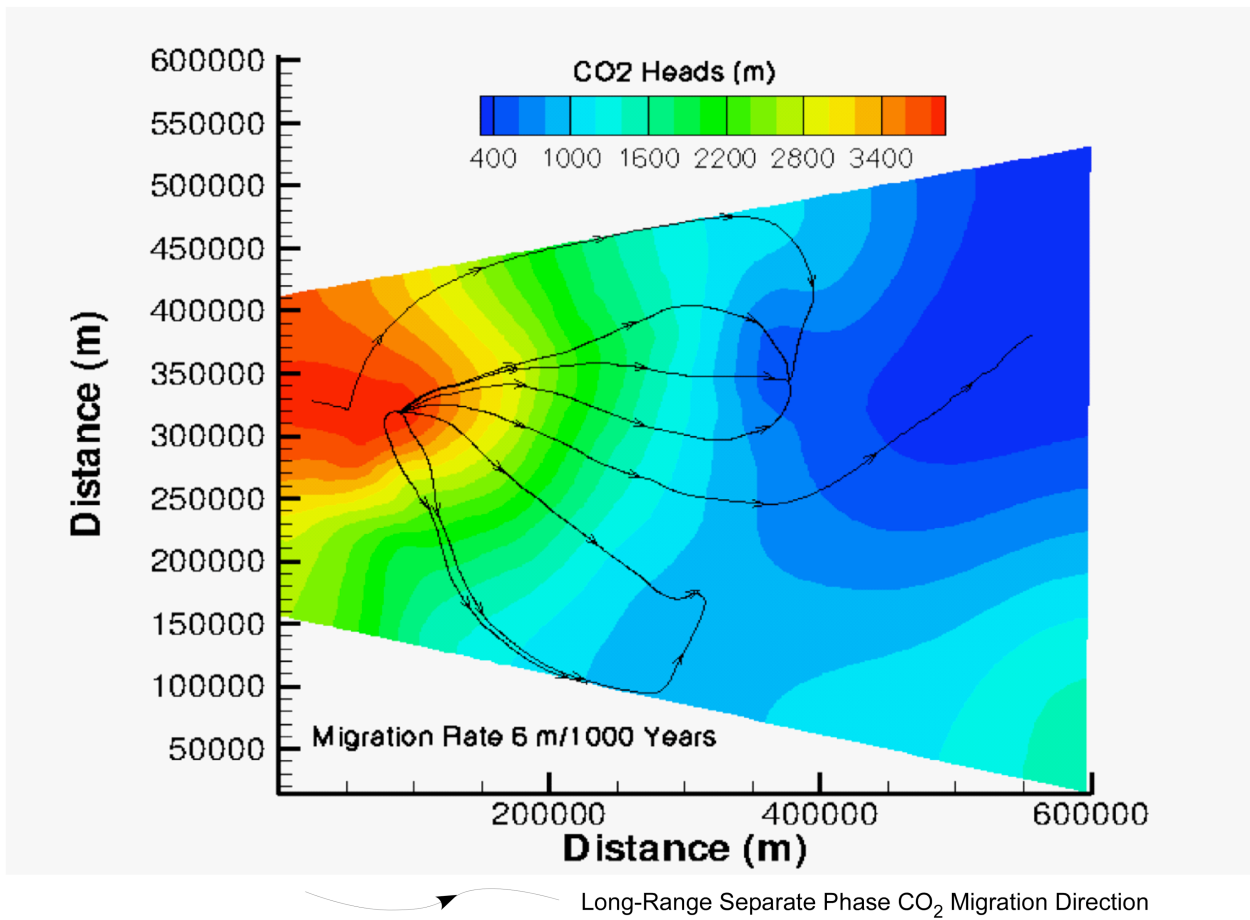


Figure 21

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Figure 22